



## Full wwPDB EM Validation Report ⓘ

May 5, 2026 – 08:40 pm BST

PDB ID : 9R78 / pdb\_00009r78  
EMDB ID : EMD-53736  
Title : Human Adenovirus D 10 Capsid Structure  
Authors : Waraich, K.; Mundy, R.M.; Bates, E.A.; da Fonseca, P.; Morris, E.; Rizkallah, P.J.; Baker, A.T.; Young, M.T.; Parker, A.L.; Bhella, D.  
Deposited on : 2025-05-14  
Resolution : 3.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

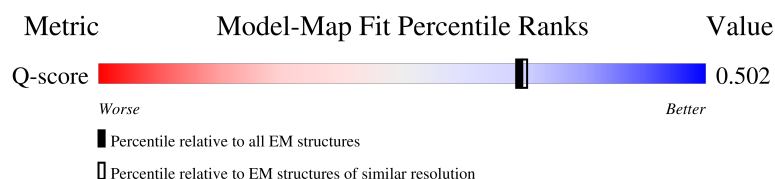
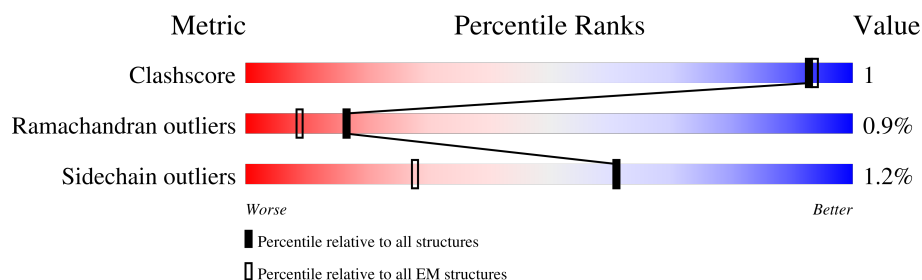
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

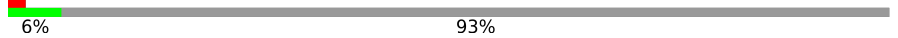
The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



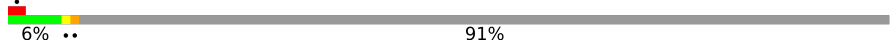
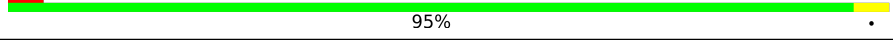
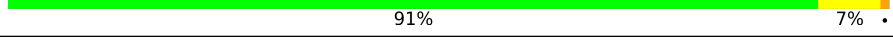
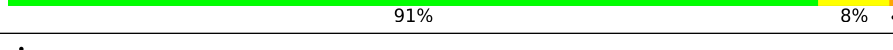
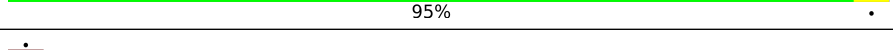
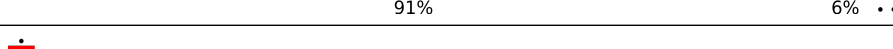
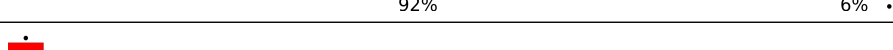
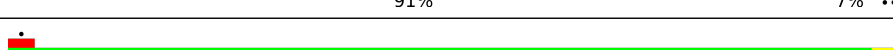
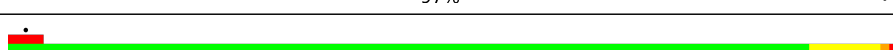
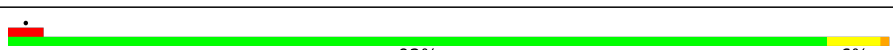
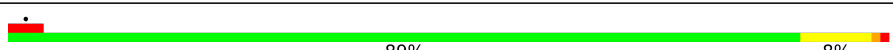
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 15087 ( 2.80 - 3.80 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | 1     | 234    |  |
| 1   | 2     | 234    |  |
| 1   | 3     | 234    |  |
| 1   | 4     | 234    |  |

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| Mol | Chain | Length | Quality of chain                                                                                |
|-----|-------|--------|-------------------------------------------------------------------------------------------------|
| 1   | 5     | 234    |  6% 89%       |
| 1   | 6     | 234    |  6% 91%       |
| 1   | 7     | 234    |  7% 88%       |
| 1   | 8     | 234    |  6% 93%       |
| 2   | A     | 941    |  95%          |
| 2   | B     | 941    |  91% 7%       |
| 2   | C     | 941    |  91% 8%       |
| 2   | D     | 941    |  95%          |
| 2   | E     | 941    |  91% 6%       |
| 2   | F     | 941    |  92% 6%       |
| 2   | G     | 941    |  91% 7%       |
| 2   | H     | 941    |  97%        |
| 2   | I     | 941    |  90% 8%     |
| 2   | J     | 941    |  96%        |
| 2   | K     | 941    |  92% 6%     |
| 2   | L     | 941    |  89% 8%     |
| 3   | M     | 519    |  87% 9%     |
| 4   | N     | 559    |  5% 48% 50% |
| 5   | O     | 227    |  72% 6% 22% |
| 5   | P     | 227    |  74% 5% 21% |
| 6   | Q     | 134    |  5% 29% 71% |
| 6   | R     | 134    |  26% 73%    |
| 6   | S     | 134    |  46% 47%    |
| 6   | T     | 134    |  7% 22% 76% |

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 198096 atoms, of which 96875 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pre-protein VI.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 1   | 1     | 22       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 340   | 112 | 163 | 33 | 31 | 1 |         |       |
| 1   | 2     | 16       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 216   | 68  | 103 | 20 | 24 | 1 |         |       |
| 1   | 3     | 21       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 325   | 107 | 157 | 32 | 28 | 1 |         |       |
| 1   | 4     | 11       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 172   | 58  | 81  | 18 | 14 | 1 |         |       |
| 1   | 5     | 25       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 393   | 128 | 191 | 36 | 36 | 2 |         |       |
| 1   | 6     | 20       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 309   | 102 | 148 | 31 | 27 | 1 |         |       |
| 1   | 7     | 27       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 415   | 134 | 204 | 39 | 37 | 1 |         |       |
| 1   | 8     | 17       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 271   | 90  | 131 | 26 | 23 | 1 |         |       |

- Molecule 2 is a protein called Hexon protein.

| Mol | Chain | Residues | Atoms |      |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|------|----|---------|-------|
| 2   | A     | 941      | Total | C    | H    | N    | O    | S  | 0       | 0     |
|     |       |          | 14639 | 4751 | 7148 | 1264 | 1441 | 35 |         |       |
| 2   | B     | 941      | Total | C    | H    | N    | O    | S  | 0       | 0     |
|     |       |          | 14639 | 4751 | 7148 | 1264 | 1441 | 35 |         |       |
| 2   | C     | 941      | Total | C    | H    | N    | O    | S  | 0       | 0     |
|     |       |          | 14640 | 4751 | 7149 | 1264 | 1441 | 35 |         |       |
| 2   | D     | 941      | Total | C    | H    | N    | O    | S  | 0       | 0     |
|     |       |          | 14640 | 4751 | 7149 | 1264 | 1441 | 35 |         |       |
| 2   | E     | 941      | Total | C    | H    | N    | O    | S  | 0       | 0     |
|     |       |          | 14639 | 4751 | 7148 | 1264 | 1441 | 35 |         |       |
| 2   | F     | 941      | Total | C    | H    | N    | O    | S  | 0       | 0     |
|     |       |          | 14639 | 4751 | 7148 | 1264 | 1441 | 35 |         |       |
| 2   | G     | 941      | Total | C    | H    | N    | O    | S  | 0       | 0     |
|     |       |          | 14640 | 4751 | 7149 | 1264 | 1441 | 35 |         |       |

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| Mol | Chain | Residues | Atoms |      |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|------|----|---------|-------|
| 2   | H     | 941      | Total | C    | H    | N    | O    | S  | 0       | 0     |
|     |       |          | 14639 | 4751 | 7148 | 1264 | 1441 | 35 |         |       |
| 2   | I     | 941      | Total | C    | H    | N    | O    | S  | 0       | 0     |
|     |       |          | 14639 | 4751 | 7148 | 1264 | 1441 | 35 |         |       |
| 2   | J     | 941      | Total | C    | H    | N    | O    | S  | 0       | 0     |
|     |       |          | 14639 | 4751 | 7148 | 1264 | 1441 | 35 |         |       |
| 2   | K     | 941      | Total | C    | H    | N    | O    | S  | 0       | 0     |
|     |       |          | 14639 | 4751 | 7148 | 1264 | 1441 | 35 |         |       |
| 2   | L     | 939      | Total | C    | H    | N    | O    | S  | 0       | 0     |
|     |       |          | 14604 | 4741 | 7129 | 1262 | 1439 | 33 |         |       |

- Molecule 3 is a protein called Penton protein.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 3   | M     | 472      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 7509  | 2410 | 3715 | 642 | 728 | 14 |         |       |

- Molecule 4 is a protein called Pre-hexon-linking protein IIIa.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 4   | N     | 281      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 4346  | 1354 | 2170 | 397 | 422 | 3 |         |       |

- Molecule 5 is a protein called Pre-hexon-linking protein VIII.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 5   | O     | 177      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2706  | 868 | 1329 | 237 | 267 | 5 |         |       |
| 5   | P     | 180      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2727  | 874 | 1338 | 240 | 270 | 5 |         |       |

- Molecule 6 is a protein called Hexon-interlacing protein.

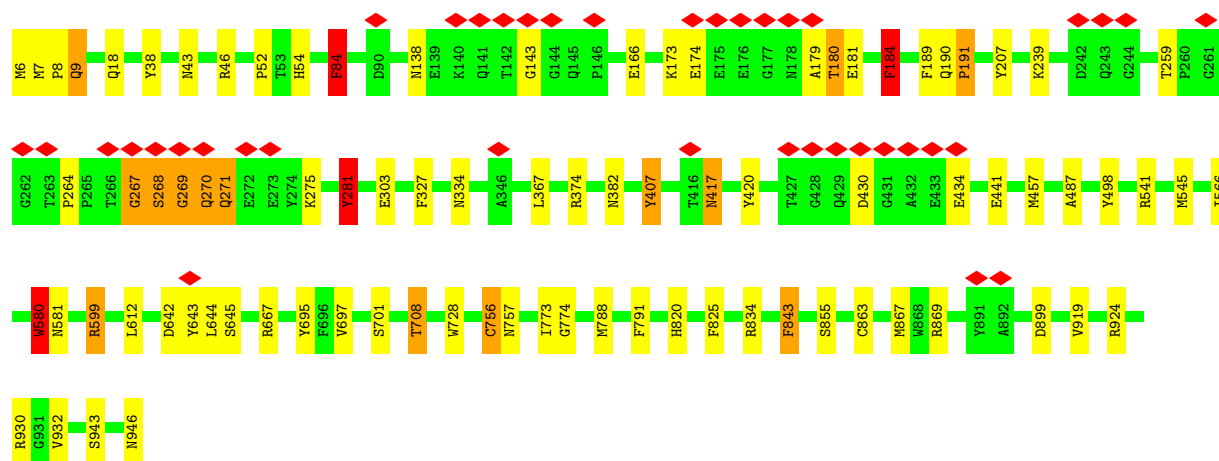
| Mol | Chain | Residues | Atoms |     |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|-----|---|---------|-------|
| 6   | Q     | 39       | Total | C   | H   | N  | O   |   | 0       | 0     |
|     |       |          | 619   | 188 | 317 | 52 | 62  |   |         |       |
| 6   | R     | 36       | Total | C   | H   | N  | O   |   | 0       | 0     |
|     |       |          | 579   | 175 | 294 | 51 | 59  |   |         |       |
| 6   | S     | 71       | Total | C   | H   | N  | O   | S | 0       | 0     |
|     |       |          | 1017  | 305 | 513 | 88 | 109 | 2 |         |       |
| 6   | T     | 32       | Total | C   | H   | N  | O   |   | 0       | 0     |
|     |       |          | 516   | 154 | 261 | 48 | 53  |   |         |       |





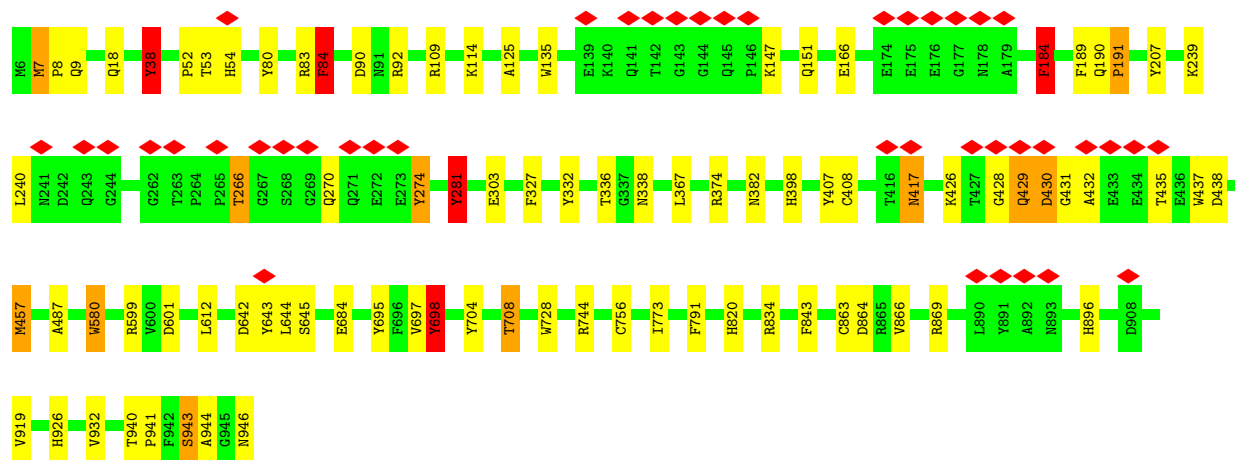






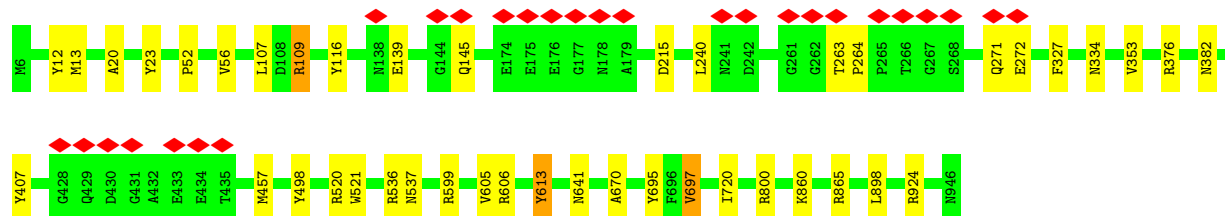
• Molecule 2: Hexon protein

Chain C: 91% 8% ..



• Molecule 2: Hexon protein

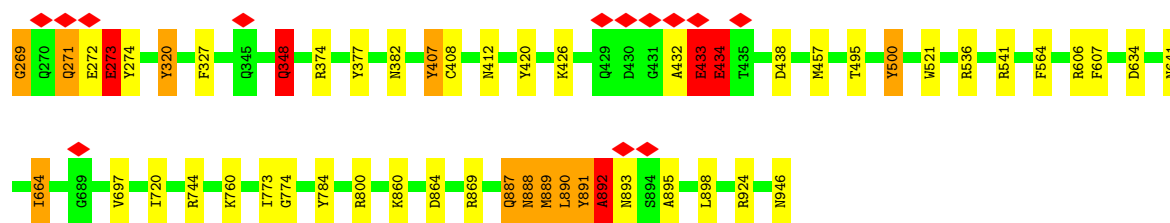
Chain D: 95% 5% .



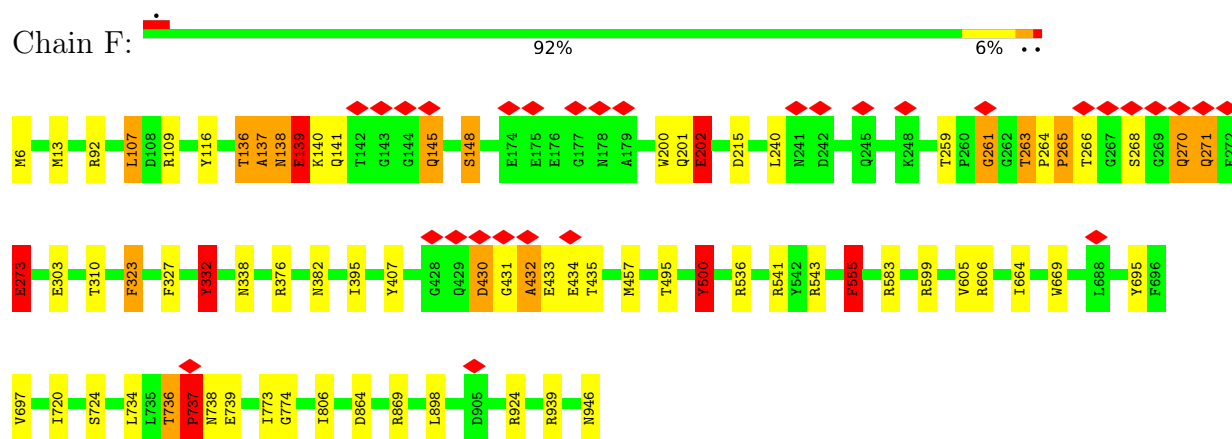
• Molecule 2: Hexon protein

Chain E: 91% 6% ..

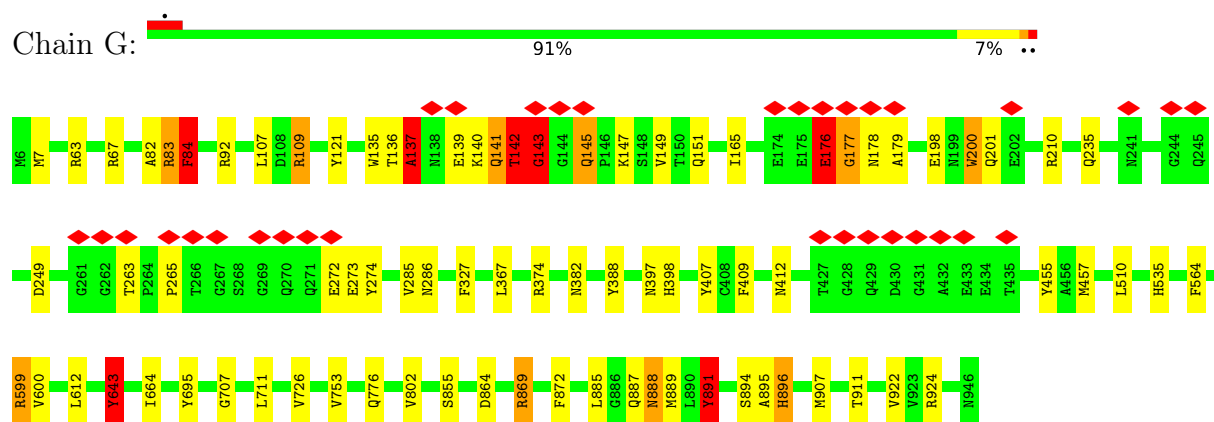




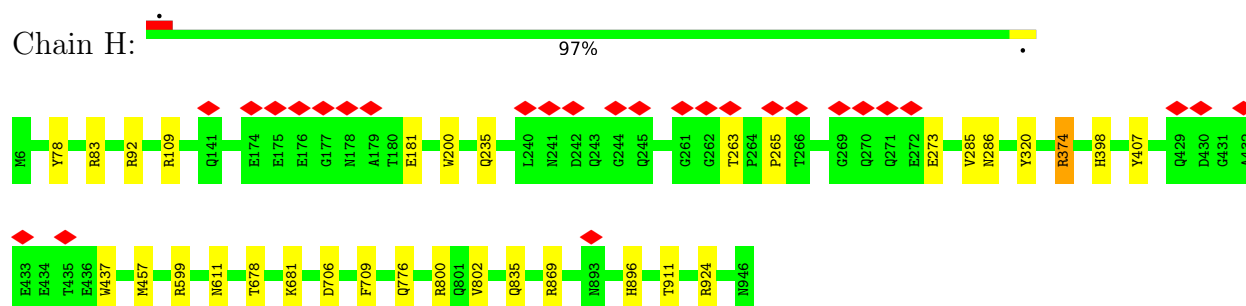
• Molecule 2: Hexon protein



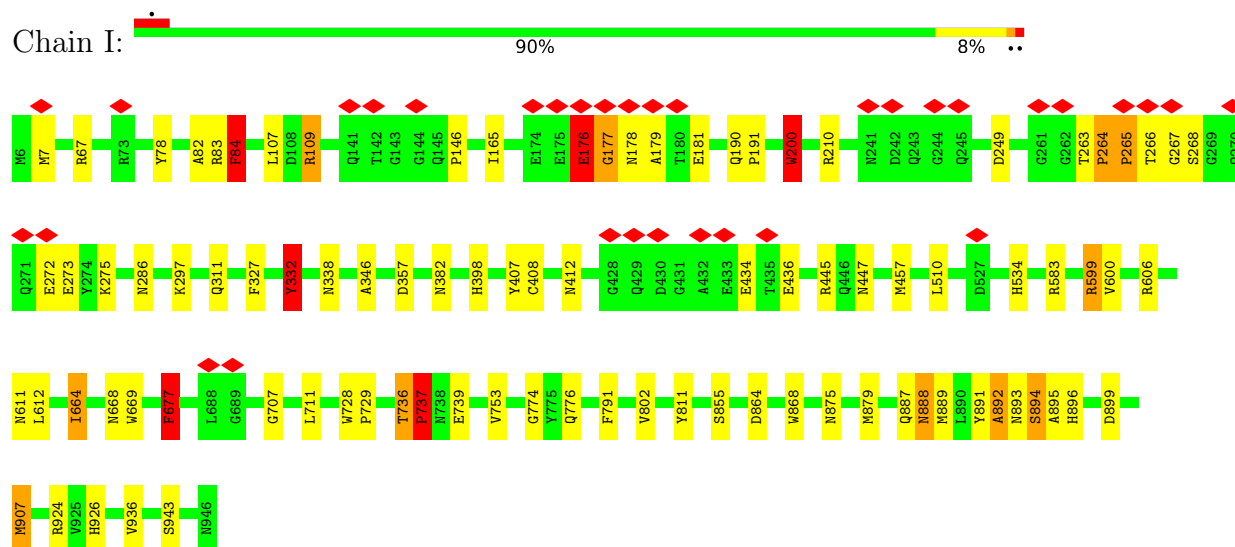
• Molecule 2: Hexon protein



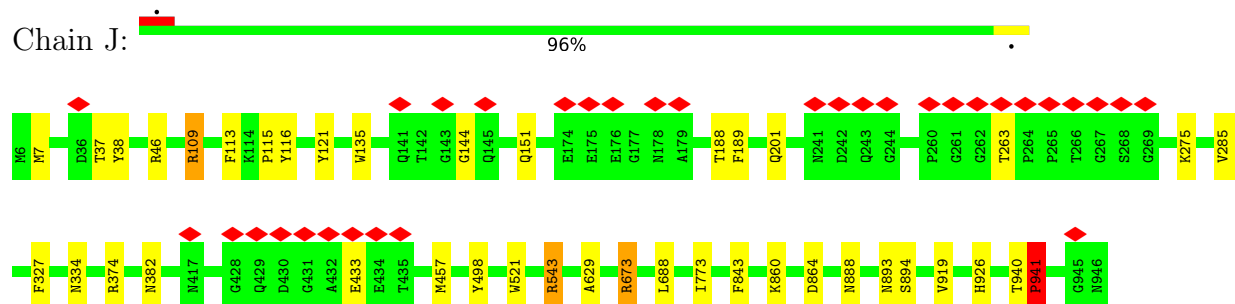
• Molecule 2: Hexon protein



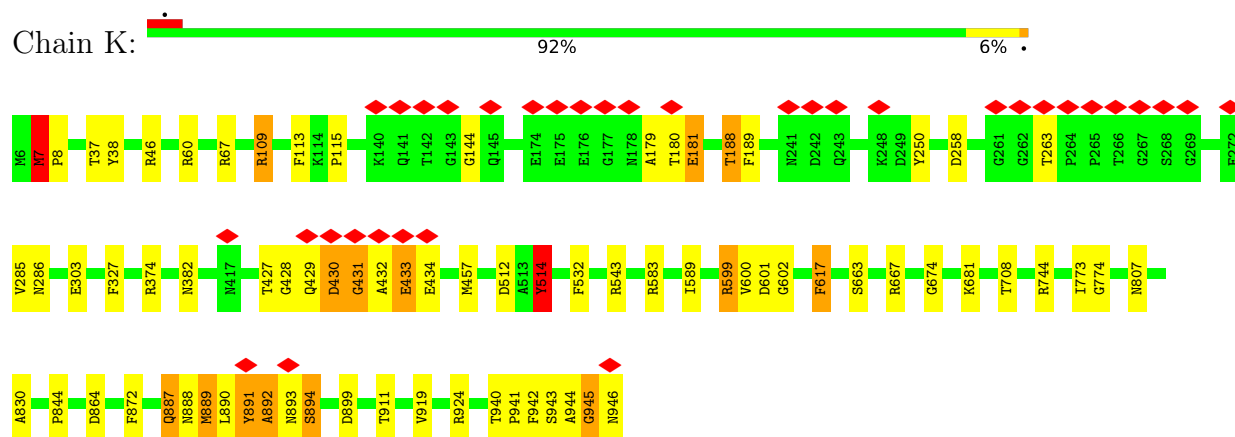
• Molecule 2: Hexon protein



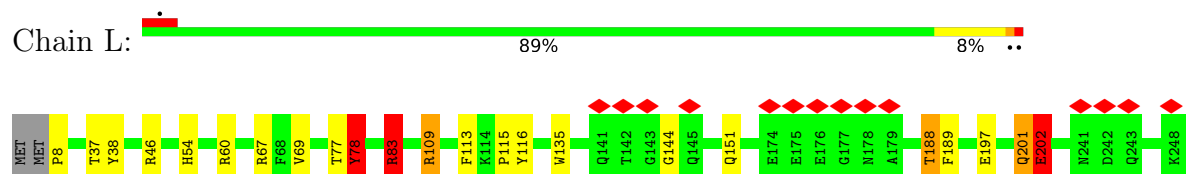
• Molecule 2: Hexon protein

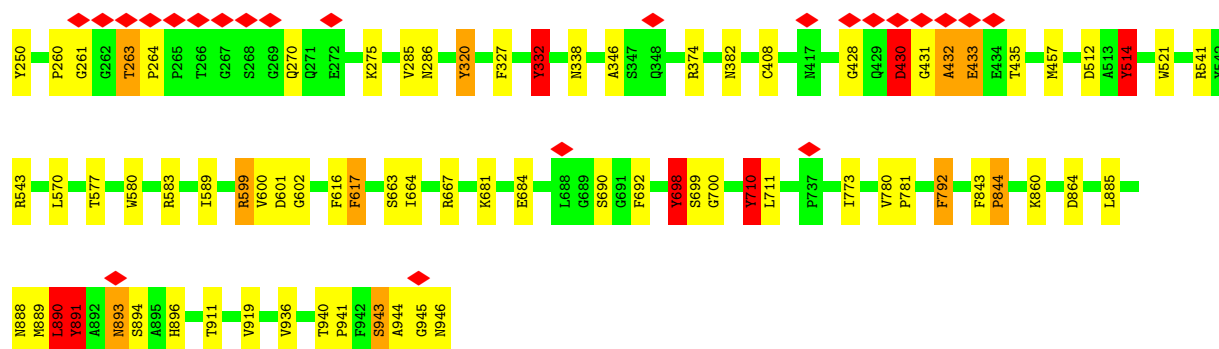


• Molecule 2: Hexon protein

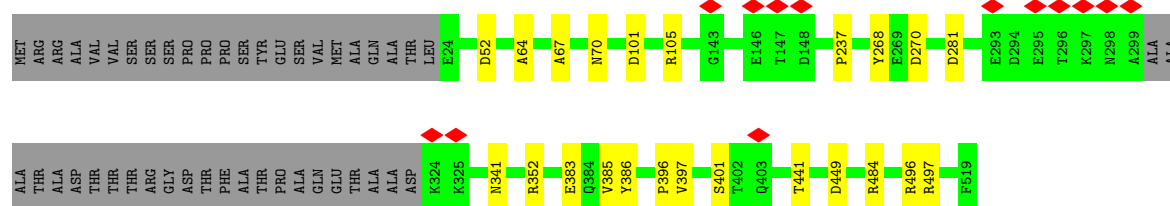


• Molecule 2: Hexon protein

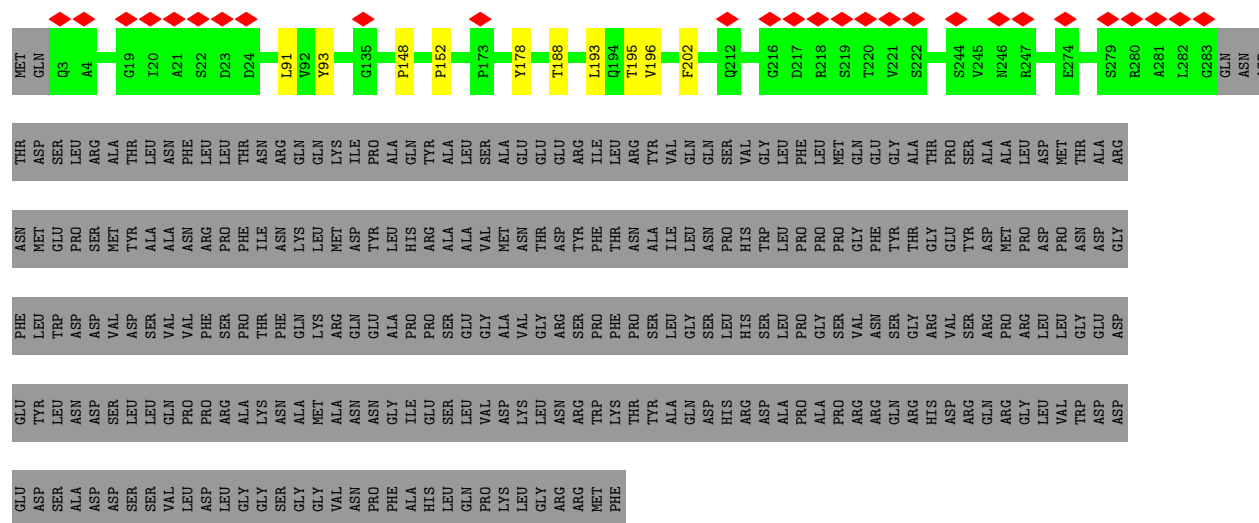




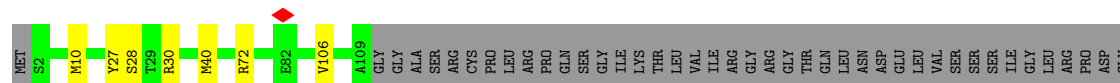
• Molecule 3: Penton protein

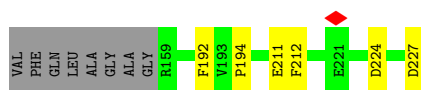


• Molecule 4: Pre-hexon-linking protein IIIa

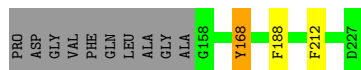
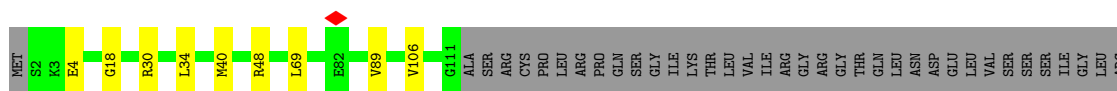


• Molecule 5: Pre-hexon-linking protein VIII

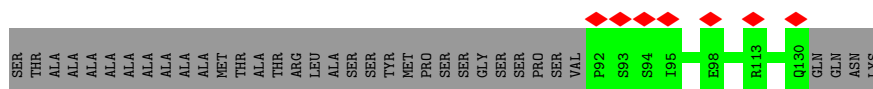
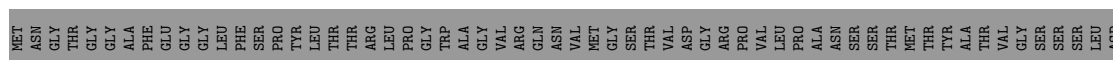




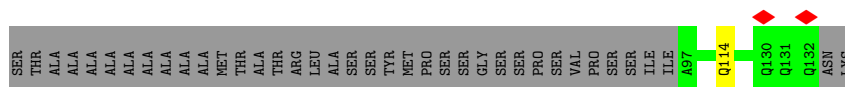
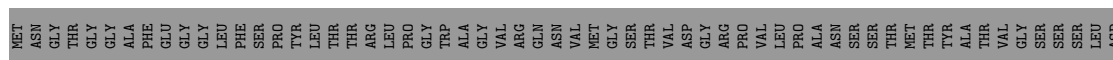
• Molecule 5: Pre-hexon-linking protein VIII



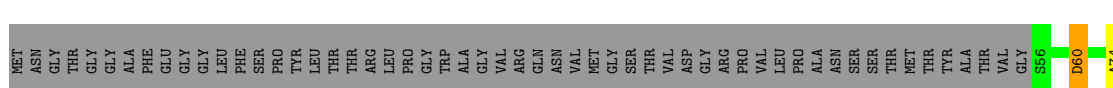
• Molecule 6: Hexon-interlacing protein



• Molecule 6: Hexon-interlacing protein



• Molecule 6: Hexon-interlacing protein



• Molecule 6: Hexon-interlacing protein



|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|
| MET | ASN | GLY | THR | GLY | GLY | ALA | PHE | GLU | GLY | GLY | LEU | PHE | SER | PRO | TYR | LEU | THR | THR | ARG | LEU | PRO | PRO | GLY | TRP | ALA | GLY | VAL | ARG | GLN | ASN | VAL | MET | GLY | SER | SER | THR | THR | ASP | GLY | ARG | PRO | VAL | VAL  | LEU  | PRO  | ALA  | ASN  | SER  | SER  | THR  | MET  | THR  | TYR  | ALA  | THR  | VAL  | GLY | SER | SER | SER | LEU | ASP |
| SER | THR | ALA | ALA | ALA | ALA | ALA | ALA | ALA | ALA | ALA | MET | THR | ALA | THR | ARG | LEU | ALA | SER | SER | TYR | PRO | MET | PRO | SER | SER | GLY | SER | SER | PRO | SER | VAL | PRO | SER | SER | ILE | ILE | ALA | GLU | GLU | LYS | LEU | LEU | A103 | L104 | L105 | A106 | E107 | R113 | Q114 | L115 | Q121 | L125 | R126 | Q132 | N133 | K134 |     |     |     |     |     |     |

## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, I                                | Depositor |
| Number of particles used             | 5524                                    | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40                                      | Depositor |
| Minimum defocus (nm)                 | 200                                     | Depositor |
| Maximum defocus (nm)                 | 2200                                    | Depositor |
| Magnification                        | 105000                                  | Depositor |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.111                                   | Depositor |
| Minimum map value                    | -0.099                                  | Depositor |
| Average map value                    | 0.003                                   | Depositor |
| Map value standard deviation         | 0.009                                   | Depositor |
| Recommended contour level            | 0.0216                                  | Depositor |
| Map size (Å)                         | 1193.76, 1193.76, 1193.76               | wwPDB     |
| Map dimensions                       | 720, 720, 720                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.658, 1.658, 1.658                     | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 1   | 1     | 1.07         | 0/183            | 1.86        | 2/248 (0.8%)      |
| 1   | 2     | 1.21         | 0/114            | 1.66        | 0/153             |
| 1   | 3     | 1.08         | 0/174            | 2.10        | 6/236 (2.5%)      |
| 1   | 4     | 0.97         | 0/95             | 2.10        | 3/128 (2.3%)      |
| 1   | 5     | 0.90         | 0/208            | 1.64        | 1/281 (0.4%)      |
| 1   | 6     | 1.15         | 0/167            | 1.70        | 1/226 (0.4%)      |
| 1   | 7     | 1.04         | 0/217            | 1.71        | 3/294 (1.0%)      |
| 1   | 8     | 1.04         | 0/144            | 1.65        | 2/193 (1.0%)      |
| 2   | A     | 0.73         | 0/7696           | 1.31        | 20/10469 (0.2%)   |
| 2   | B     | 0.85         | 12/7696 (0.2%)   | 1.51        | 72/10469 (0.7%)   |
| 2   | C     | 0.75         | 0/7696           | 1.48        | 76/10469 (0.7%)   |
| 2   | D     | 0.72         | 0/7696           | 1.29        | 12/10469 (0.1%)   |
| 2   | E     | 0.78         | 2/7696 (0.0%)    | 1.55        | 89/10469 (0.9%)   |
| 2   | F     | 0.75         | 0/7696           | 1.46        | 58/10469 (0.6%)   |
| 2   | G     | 0.74         | 0/7696           | 1.51        | 74/10469 (0.7%)   |
| 2   | H     | 0.72         | 0/7696           | 1.30        | 15/10469 (0.1%)   |
| 2   | I     | 0.74         | 0/7696           | 1.49        | 69/10469 (0.7%)   |
| 2   | J     | 0.73         | 0/7696           | 1.32        | 21/10469 (0.2%)   |
| 2   | K     | 0.75         | 0/7696           | 1.49        | 62/10469 (0.6%)   |
| 2   | L     | 0.75         | 0/7680           | 1.49        | 72/10448 (0.7%)   |
| 3   | M     | 0.74         | 0/3887           | 1.35        | 9/5290 (0.2%)     |
| 4   | N     | 0.75         | 0/2212           | 1.38        | 1/3011 (0.0%)     |
| 5   | O     | 0.77         | 0/1414           | 1.37        | 4/1929 (0.2%)     |
| 5   | P     | 0.77         | 0/1426           | 1.40        | 4/1944 (0.2%)     |
| 6   | Q     | 0.64         | 0/302            | 1.29        | 0/406             |
| 6   | R     | 0.60         | 0/284            | 1.27        | 0/381             |
| 6   | S     | 0.91         | 0/505            | 1.63        | 5/683 (0.7%)      |
| 6   | T     | 0.67         | 0/254            | 1.34        | 0/339             |
| All | All   | 0.76         | 14/103922 (0.0%) | 1.44        | 681/141349 (0.5%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.



| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | 3     | 0                   | 1                   |
| 2   | A     | 0                   | 4                   |
| 2   | B     | 0                   | 13                  |
| 2   | C     | 0                   | 14                  |
| 2   | D     | 0                   | 9                   |
| 2   | E     | 0                   | 14                  |
| 2   | F     | 0                   | 17                  |
| 2   | G     | 0                   | 16                  |
| 2   | H     | 0                   | 8                   |
| 2   | I     | 0                   | 8                   |
| 2   | J     | 0                   | 9                   |
| 2   | K     | 0                   | 11                  |
| 2   | L     | 0                   | 17                  |
| 3   | M     | 0                   | 4                   |
| 4   | N     | 0                   | 1                   |
| 5   | O     | 0                   | 3                   |
| All | All   | 0                   | 149                 |

All (14) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2   | B     | 180 | THR  | CA-CB   | -17.48 | 1.23        | 1.53     |
| 2   | B     | 180 | THR  | CB-OG1  | -16.99 | 1.16        | 1.43     |
| 2   | E     | 200 | TRP  | NE1-CE2 | -13.87 | 1.22        | 1.37     |
| 2   | B     | 180 | THR  | C-O     | -11.58 | 1.09        | 1.23     |
| 2   | B     | 181 | GLU  | CD-OE2  | -9.87  | 1.06        | 1.25     |
| 2   | B     | 179 | ALA  | C-O     | -9.33  | 1.12        | 1.24     |
| 2   | B     | 173 | LYS  | C-O     | -9.20  | 1.12        | 1.24     |
| 2   | B     | 180 | THR  | CB-CG2  | -9.14  | 1.22        | 1.52     |
| 2   | B     | 180 | THR  | CA-C    | -6.92  | 1.44        | 1.52     |
| 2   | B     | 179 | ALA  | C-N     | -6.37  | 1.25        | 1.33     |
| 2   | B     | 181 | GLU  | CG-CD   | -6.25  | 1.36        | 1.52     |
| 2   | B     | 181 | GLU  | CD-OE1  | -6.22  | 1.13        | 1.25     |
| 2   | B     | 181 | GLU  | CA-CB   | -5.31  | 1.43        | 1.54     |
| 2   | E     | 178 | ASN  | CA-C    | 5.29   | 1.59        | 1.52     |

All (681) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | E     | 179 | ALA  | N-CA-C | 22.79 | 137.12      | 112.97   |
| 2   | G     | 177 | GLY  | CA-C-N | 12.95 | 139.25      | 122.16   |
| 2   | G     | 177 | GLY  | C-N-CA | 12.95 | 139.25      | 122.16   |
| 2   | K     | 431 | GLY  | CA-C-N | 12.90 | 144.53      | 123.37   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 2   | K     | 431 | GLY  | C-N-CA      | 12.90  | 144.53      | 123.37   |
| 2   | E     | 268 | SER  | N-CA-C      | 12.62  | 131.70      | 107.98   |
| 2   | I     | 895 | ALA  | N-CA-C      | 12.57  | 129.15      | 110.30   |
| 2   | E     | 408 | CYS  | CA-CB-SG    | 12.27  | 142.61      | 114.40   |
| 2   | K     | 285 | VAL  | N-CA-C      | 11.86  | 124.97      | 113.71   |
| 2   | C     | 54  | HIS  | N-CA-C      | 11.63  | 123.95      | 111.28   |
| 2   | B     | 54  | HIS  | N-CA-C      | 11.45  | 123.77      | 111.28   |
| 2   | L     | 431 | GLY  | CA-C-N      | 11.28  | 137.90      | 122.79   |
| 2   | L     | 431 | GLY  | C-N-CA      | 11.28  | 137.90      | 122.79   |
| 2   | E     | 200 | TRP  | NE1-CE2-CD2 | -11.12 | 92.95       | 107.40   |
| 2   | G     | 895 | ALA  | N-CA-C      | 10.79  | 126.49      | 110.30   |
| 2   | B     | 268 | SER  | CA-C-N      | 10.74  | 142.47      | 121.41   |
| 2   | B     | 268 | SER  | C-N-CA      | 10.74  | 142.47      | 121.41   |
| 2   | F     | 737 | PRO  | CA-N-CD     | -10.54 | 97.25       | 112.00   |
| 2   | B     | 270 | GLN  | CA-C-N      | 10.53  | 141.66      | 121.54   |
| 2   | B     | 270 | GLN  | C-N-CA      | 10.53  | 141.66      | 121.54   |
| 2   | L     | 891 | TYR  | CB-CA-C     | 10.53  | 129.52      | 110.88   |
| 2   | F     | 737 | PRO  | CA-CB-CG    | -10.53 | 84.50       | 104.50   |
| 2   | G     | 142 | THR  | CA-CB-CG2   | 10.50  | 128.35      | 110.50   |
| 2   | L     | 943 | SER  | N-CA-C      | 10.42  | 123.23      | 108.54   |
| 2   | E     | 273 | GLU  | CB-CG-CD    | 10.39  | 130.25      | 112.60   |
| 2   | F     | 266 | THR  | N-CA-C      | -10.37 | 92.47       | 108.96   |
| 2   | L     | 201 | GLN  | CA-C-N      | 10.34  | 136.72      | 121.31   |
| 2   | L     | 201 | GLN  | C-N-CA      | 10.34  | 136.72      | 121.31   |
| 2   | B     | 184 | PHE  | CB-CG-CD2   | -10.33 | 103.14      | 120.70   |
| 2   | G     | 643 | TYR  | CB-CG-CD2   | -10.30 | 105.35      | 120.80   |
| 2   | E     | 200 | TRP  | CD1-CG-CD2  | -10.29 | 89.84       | 106.30   |
| 2   | E     | 434 | GLU  | CA-CB-CG    | 10.26  | 134.62      | 114.10   |
| 2   | B     | 773 | ILE  | N-CA-C      | 10.13  | 122.31      | 111.58   |
| 2   | F     | 201 | GLN  | CA-C-N      | 10.13  | 139.49      | 121.97   |
| 2   | F     | 201 | GLN  | C-N-CA      | 10.13  | 139.49      | 121.97   |
| 2   | C     | 698 | TYR  | CB-CG-CD2   | -10.09 | 105.66      | 120.80   |
| 2   | C     | 430 | ASP  | CA-C-N      | 9.82   | 140.66      | 121.41   |
| 2   | C     | 430 | ASP  | C-N-CA      | 9.82   | 140.66      | 121.41   |
| 2   | E     | 272 | GLU  | CA-C-N      | 9.79   | 140.23      | 121.54   |
| 2   | E     | 272 | GLU  | C-N-CA      | 9.79   | 140.23      | 121.54   |
| 2   | B     | 84  | PHE  | CB-CG-CD2   | -9.74  | 104.14      | 120.70   |
| 2   | E     | 267 | GLY  | CA-C-N      | 9.64   | 137.76      | 122.34   |
| 2   | E     | 267 | GLY  | C-N-CA      | 9.64   | 137.76      | 122.34   |
| 2   | I     | 737 | PRO  | CA-C-N      | 9.58   | 137.12      | 122.37   |
| 2   | I     | 737 | PRO  | C-N-CA      | 9.58   | 137.12      | 122.37   |
| 2   | E     | 201 | GLN  | CA-C-N      | 9.57   | 139.82      | 121.54   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | E     | 201 | GLN  | C-N-CA    | 9.57  | 139.82      | 121.54   |
| 2   | G     | 891 | TYR  | CA-C-N    | 9.44  | 139.57      | 121.54   |
| 2   | G     | 891 | TYR  | C-N-CA    | 9.44  | 139.57      | 121.54   |
| 2   | C     | 84  | PHE  | CB-CG-CD2 | -9.38 | 104.75      | 120.70   |
| 2   | G     | 142 | THR  | N-CA-CB   | -9.34 | 94.71       | 110.49   |
| 4   | N     | 202 | PHE  | CA-CB-CG  | 9.31  | 123.11      | 113.80   |
| 2   | E     | 773 | ILE  | N-CA-C    | 9.26  | 121.10      | 111.00   |
| 2   | K     | 427 | THR  | CA-C-N    | 9.22  | 133.99      | 122.83   |
| 2   | K     | 427 | THR  | C-N-CA    | 9.22  | 133.99      | 122.83   |
| 2   | I     | 177 | GLY  | CA-C-N    | 9.10  | 138.93      | 121.54   |
| 2   | I     | 177 | GLY  | C-N-CA    | 9.10  | 138.93      | 121.54   |
| 2   | B     | 774 | GLY  | N-CA-C    | 8.99  | 125.02      | 113.24   |
| 2   | C     | 184 | PHE  | CB-CG-CD2 | -8.99 | 105.42      | 120.70   |
| 2   | C     | 580 | TRP  | CB-CG-CD1 | -8.98 | 113.43      | 126.90   |
| 2   | G     | 891 | TYR  | CB-CA-C   | 8.89  | 125.52      | 111.73   |
| 2   | K     | 432 | ALA  | CA-C-N    | 8.89  | 138.52      | 121.54   |
| 2   | K     | 432 | ALA  | C-N-CA    | 8.89  | 138.52      | 121.54   |
| 2   | L     | 617 | PHE  | CA-CB-CG  | 8.84  | 122.64      | 113.80   |
| 2   | E     | 202 | GLU  | CA-CB-CG  | 8.83  | 131.76      | 114.10   |
| 2   | L     | 430 | ASP  | N-CA-C    | 8.82  | 122.54      | 112.57   |
| 2   | B     | 580 | TRP  | CB-CG-CD1 | -8.79 | 113.71      | 126.90   |
| 2   | I     | 176 | GLU  | CA-C-N    | 8.77  | 138.60      | 121.41   |
| 2   | I     | 176 | GLU  | C-N-CA    | 8.77  | 138.60      | 121.41   |
| 2   | F     | 431 | GLY  | CA-C-N    | 8.75  | 139.66      | 123.13   |
| 2   | F     | 431 | GLY  | C-N-CA    | 8.75  | 139.66      | 123.13   |
| 2   | K     | 617 | PHE  | CA-CB-CG  | 8.74  | 122.54      | 113.80   |
| 2   | K     | 428 | GLY  | CA-C-N    | 8.74  | 138.23      | 121.54   |
| 2   | K     | 428 | GLY  | C-N-CA    | 8.74  | 138.23      | 121.54   |
| 2   | G     | 891 | TYR  | CA-CB-CG  | 8.70  | 129.55      | 113.90   |
| 2   | G     | 176 | GLU  | CA-C-N    | 8.66  | 138.38      | 121.41   |
| 2   | G     | 176 | GLU  | C-N-CA    | 8.66  | 138.38      | 121.41   |
| 2   | L     | 432 | ALA  | CA-C-N    | 8.54  | 137.86      | 121.54   |
| 2   | L     | 432 | ALA  | C-N-CA    | 8.54  | 137.86      | 121.54   |
| 2   | C     | 580 | TRP  | CB-CG-CD2 | 8.53  | 138.74      | 126.80   |
| 2   | E     | 176 | GLU  | N-CA-C    | 8.50  | 123.22      | 113.02   |
| 2   | F     | 202 | GLU  | CA-CB-CG  | 8.47  | 131.04      | 114.10   |
| 2   | G     | 141 | GLN  | CA-C-N    | 8.34  | 137.46      | 121.54   |
| 2   | G     | 141 | GLN  | C-N-CA    | 8.34  | 137.46      | 121.54   |
| 2   | L     | 285 | VAL  | N-CA-C    | 8.32  | 121.62      | 113.71   |
| 2   | L     | 890 | LEU  | CA-C-N    | 8.31  | 135.30      | 122.42   |
| 2   | L     | 890 | LEU  | C-N-CA    | 8.31  | 135.30      | 122.42   |
| 2   | I     | 776 | GLN  | CA-C-N    | 8.31  | 136.65      | 121.70   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | I     | 776 | GLN  | C-N-CA     | 8.31  | 136.65      | 121.70   |
| 2   | F     | 500 | TYR  | CB-CG-CD2  | -8.28 | 108.38      | 120.80   |
| 2   | L     | 710 | TYR  | CB-CG-CD2  | -8.27 | 108.39      | 120.80   |
| 2   | I     | 664 | ILE  | CB-CA-C    | 8.23  | 118.11      | 110.13   |
| 2   | K     | 774 | GLY  | N-CA-C     | 8.22  | 122.86      | 112.83   |
| 2   | G     | 142 | THR  | N-CA-C     | 8.15  | 128.17      | 110.80   |
| 2   | F     | 737 | PRO  | CA-C-N     | -8.12 | 105.10      | 121.18   |
| 2   | F     | 737 | PRO  | C-N-CA     | -8.12 | 105.10      | 121.18   |
| 2   | B     | 180 | THR  | OG1-CB-CG2 | -8.09 | 93.12       | 109.30   |
| 2   | F     | 864 | ASP  | N-CA-C     | 8.06  | 123.15      | 113.16   |
| 2   | C     | 274 | TYR  | CA-CB-CG   | 8.01  | 128.31      | 113.90   |
| 2   | K     | 181 | GLU  | CA-CB-CG   | 7.97  | 130.04      | 114.10   |
| 2   | E     | 888 | ASN  | CA-C-N     | 7.94  | 136.71      | 121.54   |
| 2   | E     | 888 | ASN  | C-N-CA     | 7.94  | 136.71      | 121.54   |
| 2   | C     | 644 | LEU  | CA-C-N     | 7.93  | 132.01      | 120.82   |
| 2   | C     | 644 | LEU  | C-N-CA     | 7.93  | 132.01      | 120.82   |
| 2   | C     | 429 | GLN  | CA-C-N     | 7.92  | 136.67      | 121.54   |
| 2   | C     | 429 | GLN  | C-N-CA     | 7.92  | 136.67      | 121.54   |
| 2   | B     | 8   | PRO  | N-CA-C     | 7.91  | 123.94      | 113.57   |
| 2   | L     | 430 | ASP  | CA-CB-CG   | 7.91  | 120.51      | 112.60   |
| 2   | I     | 895 | ALA  | CA-C-N     | 7.88  | 132.70      | 121.42   |
| 2   | I     | 895 | ALA  | C-N-CA     | 7.88  | 132.70      | 121.42   |
| 2   | G     | 895 | ALA  | CA-C-N     | 7.84  | 132.63      | 121.42   |
| 2   | G     | 895 | ALA  | C-N-CA     | 7.84  | 132.63      | 121.42   |
| 2   | E     | 143 | GLY  | N-CA-C     | -7.80 | 94.69       | 113.18   |
| 2   | H     | 776 | GLN  | CA-C-N     | 7.79  | 135.73      | 121.70   |
| 2   | H     | 776 | GLN  | C-N-CA     | 7.79  | 135.73      | 121.70   |
| 3   | M     | 70  | ASN  | CA-CB-CG   | 7.78  | 120.38      | 112.60   |
| 2   | E     | 434 | GLU  | CB-CA-C    | -7.77 | 94.97       | 110.42   |
| 2   | C     | 728 | TRP  | N-CA-C     | 7.74  | 122.73      | 112.35   |
| 2   | C     | 274 | TYR  | CB-CA-C    | -7.73 | 97.07       | 110.45   |
| 2   | L     | 698 | TYR  | CB-CG-CD2  | -7.68 | 109.28      | 120.80   |
| 2   | G     | 200 | TRP  | CD1-CG-CD2 | -7.67 | 94.02       | 106.30   |
| 2   | L     | 332 | TYR  | CB-CG-CD2  | -7.67 | 109.30      | 120.80   |
| 2   | G     | 776 | GLN  | CA-C-N     | 7.66  | 135.50      | 121.70   |
| 2   | G     | 776 | GLN  | C-N-CA     | 7.66  | 135.50      | 121.70   |
| 2   | B     | 834 | ARG  | NE-CZ-NH2  | 7.65  | 126.08      | 119.20   |
| 2   | E     | 180 | THR  | CA-CB-CG2  | 7.61  | 123.44      | 110.50   |
| 2   | G     | 140 | LYS  | CA-C-N     | 7.61  | 136.08      | 121.54   |
| 2   | G     | 140 | LYS  | C-N-CA     | 7.61  | 136.08      | 121.54   |
| 2   | F     | 332 | TYR  | CB-CG-CD2  | -7.59 | 109.41      | 120.80   |
| 2   | A     | 834 | ARG  | NE-CZ-NH2  | 7.56  | 126.00      | 119.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | B     | 580 | TRP  | CB-CG-CD2  | 7.52  | 137.33      | 126.80   |
| 2   | B     | 728 | TRP  | N-CA-C     | 7.52  | 122.43      | 112.35   |
| 2   | A     | 644 | LEU  | CA-C-N     | 7.52  | 131.80      | 121.05   |
| 2   | A     | 644 | LEU  | C-N-CA     | 7.52  | 131.80      | 121.05   |
| 2   | E     | 864 | ASP  | N-CA-C     | 7.52  | 122.64      | 113.17   |
| 2   | K     | 773 | ILE  | N-CA-C     | 7.51  | 118.43      | 112.12   |
| 2   | E     | 268 | SER  | CA-C-O     | -7.48 | 113.20      | 121.58   |
| 2   | F     | 430 | ASP  | N-CA-C     | 7.42  | 126.61      | 110.80   |
| 2   | F     | 773 | ILE  | N-CA-C     | 7.39  | 119.05      | 111.00   |
| 2   | E     | 145 | GLN  | N-CA-C     | 7.38  | 122.39      | 109.48   |
| 2   | I     | 896 | HIS  | N-CA-C     | 7.37  | 121.84      | 110.20   |
| 2   | K     | 943 | SER  | N-CA-C     | 7.34  | 126.44      | 110.80   |
| 2   | B     | 791 | PHE  | N-CA-C     | 7.33  | 118.96      | 110.97   |
| 2   | C     | 834 | ARG  | NE-CZ-NH2  | 7.27  | 125.74      | 119.20   |
| 2   | C     | 191 | PRO  | N-CA-CB    | 7.26  | 107.59      | 102.65   |
| 2   | L     | 617 | PHE  | CB-CA-C    | 7.25  | 121.77      | 109.82   |
| 2   | K     | 181 | GLU  | N-CA-CB    | -7.24 | 100.50      | 110.42   |
| 2   | C     | 84  | PHE  | CA-CB-CG   | 7.23  | 121.03      | 113.80   |
| 2   | L     | 78  | TYR  | CB-CG-CD2  | -7.22 | 109.97      | 120.80   |
| 2   | I     | 200 | TRP  | CD1-CG-CD2 | -7.21 | 94.77       | 106.30   |
| 2   | B     | 191 | PRO  | N-CA-CB    | 7.21  | 107.47      | 102.35   |
| 2   | K     | 60  | ARG  | CB-CG-CD   | 7.15  | 127.75      | 111.30   |
| 2   | J     | 285 | VAL  | N-CA-C     | 7.11  | 120.46      | 113.71   |
| 2   | G     | 137 | ALA  | O-C-N      | -7.06 | 113.20      | 122.59   |
| 2   | I     | 707 | GLY  | N-CA-C     | -7.05 | 98.97       | 110.95   |
| 2   | I     | 263 | THR  | CA-C-N     | 7.05  | 127.64      | 120.38   |
| 2   | I     | 263 | THR  | C-N-CA     | 7.05  | 127.64      | 120.38   |
| 2   | L     | 428 | GLY  | CA-C-N     | 7.01  | 134.00      | 121.66   |
| 2   | L     | 428 | GLY  | C-N-CA     | 7.01  | 134.00      | 121.66   |
| 2   | D     | 264 | PRO  | N-CA-CB    | 7.00  | 107.11      | 103.19   |
| 2   | G     | 274 | TYR  | N-CA-C     | 6.97  | 120.42      | 109.96   |
| 2   | I     | 677 | PHE  | CB-CG-CD2  | -6.97 | 108.85      | 120.70   |
| 2   | B     | 6   | MET  | CA-C-N     | 6.97  | 128.80      | 120.09   |
| 2   | B     | 6   | MET  | C-N-CA     | 6.97  | 128.80      | 120.09   |
| 2   | K     | 945 | GLY  | CA-C-N     | 6.97  | 134.24      | 121.70   |
| 2   | K     | 945 | GLY  | C-N-CA     | 6.97  | 134.24      | 121.70   |
| 2   | E     | 142 | THR  | CB-CA-C    | 6.93  | 124.21      | 110.42   |
| 2   | K     | 617 | PHE  | CB-CA-C    | 6.92  | 121.25      | 109.82   |
| 2   | B     | 84  | PHE  | CA-CB-CG   | 6.92  | 120.72      | 113.80   |
| 2   | G     | 200 | TRP  | N-CA-C     | 6.89  | 120.78      | 112.38   |
| 2   | K     | 892 | ALA  | CA-C-O     | -6.87 | 113.42      | 120.84   |
| 2   | E     | 408 | CYS  | N-CA-CB    | -6.86 | 98.94       | 110.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | L     | 144 | GLY  | CA-C-N     | 6.85  | 127.43      | 119.83   |
| 2   | L     | 144 | GLY  | C-N-CA     | 6.85  | 127.43      | 119.83   |
| 5   | O     | 227 | ASP  | CA-CB-CG   | 6.85  | 119.45      | 112.60   |
| 2   | B     | 946 | ASN  | CA-CB-CG   | 6.83  | 119.43      | 112.60   |
| 2   | K     | 188 | THR  | CA-C-N     | 6.82  | 133.97      | 121.70   |
| 2   | K     | 188 | THR  | C-N-CA     | 6.82  | 133.97      | 121.70   |
| 2   | J     | 37  | THR  | N-CA-C     | -6.80 | 96.56       | 108.20   |
| 2   | K     | 434 | GLU  | N-CA-CB    | -6.80 | 100.11      | 110.45   |
| 2   | E     | 774 | GLY  | N-CA-C     | 6.79  | 120.86      | 112.64   |
| 2   | E     | 144 | GLY  | N-CA-C     | 6.77  | 132.94      | 113.30   |
| 1   | 4     | 19  | MET  | CA-C-N     | 6.77  | 130.97      | 121.22   |
| 1   | 4     | 19  | MET  | C-N-CA     | 6.77  | 130.97      | 121.22   |
| 2   | E     | 142 | THR  | CA-CB-CG2  | 6.77  | 122.01      | 110.50   |
| 2   | E     | 426 | LYS  | N-CA-C     | 6.76  | 118.34      | 110.97   |
| 2   | E     | 176 | GLU  | CA-CB-CG   | 6.76  | 127.61      | 114.10   |
| 2   | E     | 606 | ARG  | NE-CZ-NH2  | 6.75  | 125.28      | 119.20   |
| 2   | L     | 664 | ILE  | CB-CA-C    | 6.75  | 116.68      | 110.13   |
| 2   | L     | 188 | THR  | CA-C-N     | 6.74  | 133.84      | 121.70   |
| 2   | L     | 188 | THR  | C-N-CA     | 6.74  | 133.84      | 121.70   |
| 2   | E     | 179 | ALA  | N-CA-CB    | -6.72 | 101.11      | 110.65   |
| 2   | E     | 174 | GLU  | CA-C-O     | -6.72 | 113.95      | 121.00   |
| 2   | E     | 145 | GLN  | OE1-CD-NE2 | -6.69 | 115.91      | 122.60   |
| 2   | I     | 855 | SER  | N-CA-C     | 6.68  | 120.42      | 109.06   |
| 2   | G     | 707 | GLY  | N-CA-C     | -6.68 | 99.60       | 110.95   |
| 2   | D     | 272 | GLU  | CA-C-N     | 6.66  | 131.25      | 120.60   |
| 2   | D     | 272 | GLU  | C-N-CA     | 6.66  | 131.25      | 120.60   |
| 2   | F     | 555 | PHE  | CA-CB-CG   | 6.66  | 120.46      | 113.80   |
| 2   | C     | 7   | MET  | N-CA-C     | 6.65  | 122.75      | 113.57   |
| 2   | B     | 52  | PRO  | N-CA-C     | 6.65  | 122.56      | 113.98   |
| 2   | K     | 144 | GLY  | CA-C-N     | 6.65  | 127.21      | 119.83   |
| 2   | K     | 144 | GLY  | C-N-CA     | 6.65  | 127.21      | 119.83   |
| 2   | I     | 332 | TYR  | CB-CG-CD2  | -6.65 | 110.83      | 120.80   |
| 2   | L     | 83  | ARG  | CB-CG-CD   | 6.65  | 126.59      | 111.30   |
| 2   | B     | 599 | ARG  | NE-CZ-NH2  | 6.62  | 125.16      | 119.20   |
| 2   | I     | 264 | PRO  | CA-C-N     | 6.62  | 128.11      | 119.84   |
| 2   | I     | 264 | PRO  | C-N-CA     | 6.62  | 128.11      | 119.84   |
| 2   | C     | 428 | GLY  | CA-C-N     | 6.61  | 132.39      | 122.67   |
| 2   | C     | 428 | GLY  | C-N-CA     | 6.61  | 132.39      | 122.67   |
| 2   | I     | 891 | TYR  | N-CA-C     | -6.59 | 96.30       | 108.24   |
| 2   | K     | 887 | GLN  | CA-C-N     | 6.59  | 132.22      | 122.86   |
| 2   | K     | 887 | GLN  | C-N-CA     | 6.59  | 132.22      | 122.86   |
| 2   | B     | 644 | LEU  | CA-C-N     | 6.59  | 130.47      | 121.05   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | B     | 644 | LEU  | C-N-CA     | 6.59  | 130.47      | 121.05   |
| 2   | F     | 737 | PRO  | N-CA-C     | 6.56  | 125.99      | 112.47   |
| 2   | J     | 188 | THR  | CA-C-N     | 6.56  | 133.51      | 121.70   |
| 2   | J     | 188 | THR  | C-N-CA     | 6.56  | 133.51      | 121.70   |
| 2   | F     | 271 | GLN  | CA-C-N     | 6.56  | 135.06      | 121.94   |
| 2   | F     | 271 | GLN  | C-N-CA     | 6.56  | 135.06      | 121.94   |
| 2   | L     | 698 | TYR  | CA-CB-CG   | 6.55  | 125.68      | 113.90   |
| 2   | K     | 7   | MET  | CA-CB-CG   | 6.54  | 127.19      | 114.10   |
| 2   | A     | 599 | ARG  | NE-CZ-NH2  | 6.54  | 125.09      | 119.20   |
| 2   | B     | 756 | CYS  | N-CA-CB    | -6.53 | 101.40      | 111.46   |
| 2   | K     | 430 | ASP  | CA-CB-CG   | 6.53  | 119.13      | 112.60   |
| 2   | A     | 52  | PRO  | N-CA-C     | 6.53  | 122.03      | 114.20   |
| 2   | C     | 240 | LEU  | N-CA-C     | 6.53  | 120.92      | 113.15   |
| 2   | G     | 896 | HIS  | N-CA-C     | 6.52  | 120.51      | 110.20   |
| 2   | L     | 202 | GLU  | CA-CB-CG   | 6.52  | 127.14      | 114.10   |
| 2   | I     | 408 | CYS  | CA-CB-SG   | 6.51  | 129.38      | 114.40   |
| 2   | I     | 600 | VAL  | N-CA-C     | -6.51 | 101.14      | 109.80   |
| 2   | C     | 281 | TYR  | CB-CG-CD2  | -6.50 | 111.05      | 120.80   |
| 2   | I     | 774 | GLY  | N-CA-C     | 6.49  | 122.07      | 113.37   |
| 2   | C     | 599 | ARG  | NE-CZ-NH2  | 6.48  | 125.03      | 119.20   |
| 2   | F     | 500 | TYR  | CD1-CG-CD2 | -6.48 | 108.38      | 118.10   |
| 2   | G     | 149 | VAL  | CB-CA-C    | -6.47 | 104.20      | 111.45   |
| 2   | E     | 433 | GLU  | CA-C-N     | -6.47 | 109.19      | 121.54   |
| 2   | E     | 433 | GLU  | C-N-CA     | -6.47 | 109.19      | 121.54   |
| 2   | B     | 788 | MET  | N-CA-C     | 6.46  | 118.32      | 111.28   |
| 2   | C     | 698 | TYR  | N-CA-C     | 6.44  | 119.10      | 108.99   |
| 2   | C     | 773 | ILE  | N-CA-C     | 6.44  | 118.02      | 111.00   |
| 2   | I     | 753 | VAL  | CB-CA-C    | -6.44 | 100.41      | 110.52   |
| 2   | E     | 200 | TRP  | CG-CD2-CE3 | -6.42 | 127.48      | 133.90   |
| 2   | B     | 180 | THR  | N-CA-C     | 6.41  | 119.07      | 110.35   |
| 2   | K     | 602 | GLY  | N-CA-C     | 6.41  | 124.53      | 115.30   |
| 2   | E     | 434 | GLU  | CA-C-N     | 6.41  | 134.87      | 123.34   |
| 2   | E     | 434 | GLU  | C-N-CA     | 6.41  | 134.87      | 123.34   |
| 2   | G     | 143 | GLY  | O-C-N      | -6.40 | 114.37      | 122.70   |
| 2   | F     | 136 | THR  | O-C-N      | -6.39 | 113.80      | 122.94   |
| 2   | I     | 445 | ARG  | NE-CZ-NH2  | 6.39  | 124.95      | 119.20   |
| 2   | G     | 145 | GLN  | N-CA-C     | 6.38  | 118.57      | 108.23   |
| 2   | F     | 136 | THR  | CA-C-N     | -6.37 | 109.37      | 121.54   |
| 2   | F     | 136 | THR  | C-N-CA     | -6.37 | 109.37      | 121.54   |
| 2   | C     | 53  | THR  | CA-CB-CG2  | 6.36  | 121.32      | 110.50   |
| 2   | F     | 738 | ASN  | N-CA-C     | -6.36 | 105.38      | 113.01   |
| 2   | G     | 600 | VAL  | N-CA-C     | -6.35 | 101.35      | 109.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | B     | 843 | PHE  | N-CA-C      | 6.35  | 123.83      | 109.81   |
| 2   | E     | 18  | GLN  | N-CA-C      | 6.34  | 119.80      | 109.59   |
| 2   | B     | 7   | MET  | N-CA-C      | 6.34  | 122.16      | 113.16   |
| 2   | E     | 269 | GLY  | CA-C-N      | 6.33  | 133.63      | 121.54   |
| 2   | E     | 269 | GLY  | C-N-CA      | 6.33  | 133.63      | 121.54   |
| 3   | M     | 496 | ARG  | NE-CZ-NH2   | 6.33  | 124.90      | 119.20   |
| 2   | K     | 109 | ARG  | NE-CZ-NH2   | 6.33  | 124.89      | 119.20   |
| 2   | E     | 54  | HIS  | N-CA-C      | 6.32  | 120.84      | 111.04   |
| 2   | F     | 137 | ALA  | CA-C-N      | 6.32  | 133.61      | 121.54   |
| 2   | F     | 137 | ALA  | C-N-CA      | 6.32  | 133.61      | 121.54   |
| 2   | B     | 281 | TYR  | CB-CG-CD2   | -6.32 | 111.33      | 120.80   |
| 2   | L     | 896 | HIS  | CB-CG-CD2   | -6.31 | 123.00      | 131.20   |
| 2   | C     | 728 | TRP  | CB-CA-C     | -6.31 | 102.76      | 113.04   |
| 2   | K     | 430 | ASP  | N-CA-C      | 6.30  | 122.06      | 113.37   |
| 1   | 3     | 18  | PHE  | CA-C-N      | 6.30  | 133.56      | 121.54   |
| 1   | 3     | 18  | PHE  | C-N-CA      | 6.30  | 133.56      | 121.54   |
| 2   | J     | 773 | ILE  | N-CA-C      | 6.29  | 117.40      | 112.12   |
| 2   | E     | 887 | GLN  | CA-C-N      | 6.29  | 133.55      | 121.54   |
| 2   | E     | 887 | GLN  | C-N-CA      | 6.29  | 133.55      | 121.54   |
| 2   | B     | 487 | ALA  | N-CA-C      | 6.29  | 118.94      | 111.71   |
| 2   | E     | 200 | TRP  | CE2-CD2-CE3 | -6.29 | 112.51      | 118.80   |
| 2   | F     | 432 | ALA  | CA-C-N      | 6.27  | 133.52      | 121.54   |
| 2   | F     | 432 | ALA  | C-N-CA      | 6.27  | 133.52      | 121.54   |
| 2   | G     | 84  | PHE  | CD1-CG-CD2  | -6.27 | 109.19      | 118.60   |
| 2   | C     | 18  | GLN  | N-CA-C      | 6.27  | 118.87      | 110.35   |
| 2   | L     | 888 | ASN  | CA-C-N      | 6.26  | 133.50      | 121.54   |
| 2   | L     | 888 | ASN  | C-N-CA      | 6.26  | 133.50      | 121.54   |
| 2   | B     | 264 | PRO  | N-CA-C      | -6.26 | 103.88      | 110.58   |
| 2   | F     | 136 | THR  | N-CA-C      | -6.24 | 100.26      | 109.81   |
| 2   | G     | 139 | GLU  | N-CA-C      | 6.24  | 119.57      | 109.40   |
| 2   | G     | 147 | LYS  | N-CA-C      | 6.23  | 120.96      | 113.23   |
| 2   | E     | 109 | ARG  | NE-CZ-NH2   | 6.22  | 124.80      | 119.20   |
| 2   | G     | 643 | TYR  | CD1-CG-CD2  | -6.21 | 108.78      | 118.10   |
| 2   | F     | 264 | PRO  | N-CA-CB     | 6.20  | 109.09      | 103.08   |
| 2   | C     | 791 | PHE  | N-CA-C      | 6.19  | 117.72      | 110.97   |
| 2   | B     | 932 | VAL  | N-CA-C      | 6.19  | 119.18      | 108.90   |
| 2   | B     | 190 | GLN  | N-CA-C      | 6.17  | 122.09      | 113.57   |
| 2   | L     | 37  | THR  | N-CA-C      | -6.17 | 98.67       | 108.73   |
| 2   | C     | 698 | TYR  | CA-CB-CG    | 6.15  | 124.98      | 113.90   |
| 2   | L     | 602 | GLY  | N-CA-C      | 6.15  | 124.15      | 115.30   |
| 2   | F     | 395 | ILE  | N-CA-C      | 6.14  | 117.62      | 110.62   |
| 2   | E     | 272 | GLU  | CA-CB-CG    | 6.13  | 126.35      | 114.10   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | E     | 147 | LYS  | N-CA-C    | 6.12  | 118.75      | 111.71   |
| 2   | G     | 145 | GLN  | CA-C-N    | 6.11  | 126.02      | 119.85   |
| 2   | G     | 145 | GLN  | C-N-CA    | 6.11  | 126.02      | 119.85   |
| 2   | E     | 892 | ALA  | CA-C-N    | 6.11  | 129.30      | 120.38   |
| 2   | E     | 892 | ALA  | C-N-CA    | 6.11  | 129.30      | 120.38   |
| 2   | I     | 599 | ARG  | N-CA-C    | -6.10 | 104.55      | 111.14   |
| 2   | D     | 109 | ARG  | NE-CZ-NH2 | 6.09  | 124.68      | 119.20   |
| 3   | M     | 352 | ARG  | NE-CZ-NH2 | 6.08  | 124.67      | 119.20   |
| 1   | 1     | 5   | ASN  | CA-CB-CG  | 6.07  | 118.67      | 112.60   |
| 2   | L     | 698 | TYR  | CB-CG-CD1 | 6.07  | 129.91      | 120.80   |
| 2   | I     | 249 | ASP  | N-CA-C    | 6.06  | 118.63      | 109.41   |
| 2   | E     | 176 | GLU  | O-C-N     | -6.05 | 114.58      | 122.39   |
| 2   | F     | 924 | ARG  | NE-CZ-NH2 | 6.05  | 124.64      | 119.20   |
| 2   | B     | 834 | ARG  | CD-NE-CZ  | 6.04  | 132.86      | 124.40   |
| 2   | D     | 924 | ARG  | NE-CZ-NH2 | 6.04  | 124.63      | 119.20   |
| 2   | L     | 109 | ARG  | NE-CZ-NH2 | 6.04  | 124.63      | 119.20   |
| 2   | L     | 37  | THR  | CA-C-N    | 6.03  | 132.56      | 121.70   |
| 2   | L     | 37  | THR  | C-N-CA    | 6.03  | 132.56      | 121.70   |
| 2   | J     | 144 | GLY  | CA-C-N    | 6.02  | 126.52      | 119.83   |
| 2   | J     | 144 | GLY  | C-N-CA    | 6.02  | 126.52      | 119.83   |
| 2   | F     | 273 | GLU  | N-CA-C    | 6.02  | 123.62      | 110.80   |
| 2   | C     | 834 | ARG  | CD-NE-CZ  | 6.01  | 132.82      | 124.40   |
| 2   | F     | 555 | PHE  | CB-CG-CD2 | -6.01 | 110.48      | 120.70   |
| 2   | G     | 753 | VAL  | CB-CA-C   | -6.01 | 101.08      | 110.52   |
| 2   | I     | 200 | TRP  | N-CA-C    | 6.01  | 120.08      | 112.87   |
| 2   | E     | 19  | ASP  | CA-CB-CG  | 5.99  | 118.59      | 112.60   |
| 2   | J     | 109 | ARG  | NE-CZ-NH2 | 5.99  | 124.59      | 119.20   |
| 2   | E     | 664 | ILE  | CB-CA-C   | 5.99  | 115.94      | 110.13   |
| 3   | M     | 270 | ASP  | CA-CB-CG  | 5.97  | 118.58      | 112.60   |
| 2   | J     | 37  | THR  | CA-C-N    | 5.97  | 132.45      | 121.70   |
| 2   | J     | 37  | THR  | C-N-CA    | 5.97  | 132.45      | 121.70   |
| 2   | B     | 374 | ARG  | NE-CZ-NH2 | 5.97  | 124.57      | 119.20   |
| 2   | C     | 932 | VAL  | N-CA-C    | 5.96  | 118.80      | 108.90   |
| 2   | G     | 285 | VAL  | N-CA-C    | 5.96  | 118.88      | 113.10   |
| 2   | K     | 434 | GLU  | N-CA-C    | 5.95  | 118.59      | 110.55   |
| 1   | 6     | 6   | PHE  | N-CA-C    | 5.95  | 118.11      | 109.07   |
| 2   | L     | 891 | TYR  | N-CA-CB   | -5.95 | 99.62       | 110.27   |
| 2   | F     | 435 | THR  | N-CA-C    | 5.94  | 119.40      | 108.58   |
| 2   | E     | 895 | ALA  | CA-C-N    | -5.94 | 112.44      | 120.87   |
| 2   | E     | 895 | ALA  | C-N-CA    | -5.94 | 112.44      | 120.87   |
| 1   | 3     | 10  | ALA  | N-CA-C    | 5.93  | 122.92      | 109.81   |
| 2   | E     | 180 | THR  | N-CA-C    | 5.93  | 119.41      | 110.64   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | C     | 866 | VAL  | CB-CA-C     | -5.93 | 104.81      | 111.45   |
| 2   | A     | 54  | HIS  | N-CA-C      | 5.92  | 117.81      | 111.36   |
| 2   | C     | 698 | TYR  | CB-CG-CD1   | 5.92  | 129.68      | 120.80   |
| 2   | E     | 438 | ASP  | CA-CB-CG    | 5.92  | 118.52      | 112.60   |
| 2   | H     | 92  | ARG  | NE-CZ-NH2   | 5.91  | 124.52      | 119.20   |
| 2   | L     | 286 | ASN  | CA-CB-CG    | 5.91  | 118.51      | 112.60   |
| 2   | L     | 710 | TYR  | N-CA-CB     | -5.90 | 100.51      | 110.49   |
| 2   | L     | 943 | SER  | CA-C-N      | 5.90  | 132.32      | 121.70   |
| 2   | L     | 943 | SER  | C-N-CA      | 5.90  | 132.32      | 121.70   |
| 2   | B     | 580 | TRP  | CB-CA-C     | 5.90  | 121.36      | 109.38   |
| 2   | A     | 834 | ARG  | CD-NE-CZ    | 5.89  | 132.64      | 124.40   |
| 2   | E     | 200 | TRP  | CB-CG-CD2   | 5.88  | 135.04      | 126.80   |
| 2   | L     | 543 | ARG  | NE-CZ-NH2   | 5.88  | 124.50      | 119.20   |
| 2   | L     | 690 | SER  | N-CA-C      | -5.88 | 101.13      | 109.96   |
| 2   | A     | 46  | ARG  | NE-CZ-NH2   | 5.88  | 124.49      | 119.20   |
| 2   | C     | 109 | ARG  | NE-CZ-NH2   | 5.87  | 124.48      | 119.20   |
| 2   | C     | 207 | TYR  | CA-C-N      | 5.87  | 126.23      | 122.18   |
| 2   | C     | 207 | TYR  | C-N-CA      | 5.87  | 126.23      | 122.18   |
| 2   | E     | 180 | THR  | CB-CA-C     | -5.87 | 102.58      | 109.80   |
| 2   | B     | 930 | ARG  | CB-CG-CD    | -5.86 | 97.81       | 111.30   |
| 2   | C     | 642 | ASP  | N-CA-C      | -5.86 | 101.37      | 110.10   |
| 2   | F     | 140 | LYS  | N-CA-C      | 5.85  | 119.67      | 111.30   |
| 2   | I     | 677 | PHE  | CA-CB-CG    | 5.85  | 119.65      | 113.80   |
| 2   | E     | 271 | GLN  | CA-C-N      | 5.84  | 133.95      | 122.61   |
| 2   | E     | 271 | GLN  | C-N-CA      | 5.84  | 133.95      | 122.61   |
| 2   | B     | 9   | GLN  | OE1-CD-NE2  | -5.84 | 116.76      | 122.60   |
| 2   | L     | 428 | GLY  | N-CA-C      | 5.84  | 120.55      | 112.37   |
| 2   | G     | 397 | ASN  | N-CA-C      | 5.84  | 118.67      | 109.39   |
| 2   | L     | 188 | THR  | N-CA-C      | -5.83 | 99.68       | 109.07   |
| 2   | F     | 145 | GLN  | N-CA-C      | 5.83  | 119.69      | 109.48   |
| 2   | L     | 891 | TYR  | CD1-CG-CD2  | -5.83 | 109.35      | 118.10   |
| 2   | G     | 887 | GLN  | CA-C-N      | 5.82  | 132.66      | 121.54   |
| 2   | G     | 887 | GLN  | C-N-CA      | 5.82  | 132.66      | 121.54   |
| 2   | G     | 235 | GLN  | OE1-CD-NE2  | -5.82 | 116.78      | 122.60   |
| 2   | E     | 145 | GLN  | CG-CD-NE2   | 5.82  | 125.12      | 116.40   |
| 2   | E     | 200 | TRP  | NE1-CE2-CZ2 | -5.80 | 121.40      | 130.10   |
| 2   | K     | 37  | THR  | N-CA-C      | -5.79 | 98.31       | 108.20   |
| 2   | C     | 190 | GLN  | N-CA-C      | 5.78  | 121.55      | 113.57   |
| 2   | I     | 272 | GLU  | N-CA-C      | 5.78  | 117.92      | 108.55   |
| 2   | I     | 776 | GLN  | O-C-N       | -5.78 | 115.38      | 122.55   |
| 3   | M     | 397 | VAL  | N-CA-C      | 5.76  | 120.08      | 112.76   |
| 2   | F     | 946 | ASN  | CA-CB-CG    | 5.75  | 118.36      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | G     | 894 | SER  | CA-C-N     | 5.74  | 130.39      | 121.26   |
| 2   | G     | 894 | SER  | C-N-CA     | 5.74  | 130.39      | 121.26   |
| 2   | K     | 286 | ASN  | CA-CB-CG   | 5.74  | 118.34      | 112.60   |
| 2   | L     | 54  | HIS  | CB-CG-CD2  | -5.74 | 123.74      | 131.20   |
| 2   | E     | 374 | ARG  | NE-CZ-NH2  | 5.74  | 124.36      | 119.20   |
| 2   | F     | 939 | ARG  | NE-CZ-NH2  | 5.74  | 124.36      | 119.20   |
| 2   | G     | 726 | VAL  | N-CA-C     | 5.74  | 112.35      | 106.21   |
| 2   | I     | 611 | ASN  | CA-CB-CG   | 5.73  | 118.33      | 112.60   |
| 2   | E     | 107 | LEU  | CB-CA-C    | -5.73 | 99.81       | 109.50   |
| 2   | F     | 500 | TYR  | CB-CA-C    | 5.73  | 119.95      | 110.90   |
| 2   | H     | 924 | ARG  | NE-CZ-NH2  | 5.72  | 124.35      | 119.20   |
| 2   | E     | 178 | ASN  | CA-C-N     | 5.72  | 131.99      | 122.66   |
| 2   | E     | 178 | ASN  | C-N-CA     | 5.72  | 131.99      | 122.66   |
| 2   | G     | 888 | ASN  | N-CA-CB    | 5.72  | 120.16      | 110.49   |
| 2   | B     | 645 | SER  | N-CA-C     | 5.72  | 118.64      | 110.24   |
| 2   | C     | 84  | PHE  | CD1-CG-CD2 | -5.72 | 110.03      | 118.60   |
| 2   | F     | 270 | GLN  | O-C-N      | -5.71 | 117.50      | 123.56   |
| 6   | S     | 110 | ALA  | CA-C-N     | 5.71  | 127.86      | 120.44   |
| 6   | S     | 110 | ALA  | C-N-CA     | 5.71  | 127.86      | 120.44   |
| 2   | B     | 267 | GLY  | CA-C-N     | 5.70  | 132.43      | 121.54   |
| 2   | B     | 267 | GLY  | C-N-CA     | 5.70  | 132.43      | 121.54   |
| 2   | G     | 285 | VAL  | CA-CB-CG1  | 5.69  | 120.07      | 110.40   |
| 2   | B     | 259 | THR  | CA-C-N     | 5.69  | 126.15      | 120.52   |
| 2   | B     | 259 | THR  | C-N-CA     | 5.69  | 126.15      | 120.52   |
| 2   | A     | 774 | GLY  | N-CA-C     | 5.68  | 121.26      | 113.99   |
| 2   | K     | 943 | SER  | N-CA-CB    | -5.68 | 100.89      | 110.49   |
| 2   | F     | 259 | THR  | CA-C-N     | 5.67  | 126.93      | 119.84   |
| 2   | F     | 259 | THR  | C-N-CA     | 5.67  | 126.93      | 119.84   |
| 2   | I     | 84  | PHE  | CD1-CG-CD2 | -5.67 | 110.10      | 118.60   |
| 2   | L     | 710 | TYR  | CA-CB-CG   | 5.66  | 124.09      | 113.90   |
| 2   | E     | 433 | GLU  | O-C-N      | -5.66 | 115.83      | 123.19   |
| 2   | K     | 830 | ALA  | N-CA-C     | 5.66  | 113.31      | 108.22   |
| 2   | G     | 92  | ARG  | NE-CZ-NH2  | 5.66  | 124.29      | 119.20   |
| 2   | K     | 543 | ARG  | NE-CZ-NH2  | 5.66  | 124.29      | 119.20   |
| 2   | F     | 774 | GLY  | N-CA-C     | 5.65  | 119.06      | 112.50   |
| 2   | G     | 198 | GLU  | N-CA-C     | 5.65  | 119.35      | 112.23   |
| 2   | A     | 374 | ARG  | NE-CZ-NH2  | 5.64  | 124.27      | 119.20   |
| 2   | C     | 820 | HIS  | CB-CG-CD2  | -5.63 | 123.89      | 131.20   |
| 2   | C     | 239 | LYS  | CB-CA-C    | 5.62  | 119.03      | 109.53   |
| 2   | K     | 514 | TYR  | N-CA-CB    | -5.62 | 102.17      | 110.49   |
| 2   | L     | 83  | ARG  | NE-CZ-NH2  | 5.62  | 124.26      | 119.20   |
| 2   | G     | 210 | ARG  | NE-CZ-NH2  | 5.62  | 124.26      | 119.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | B     | 855 | SER  | N-CA-C     | 5.62  | 117.81      | 108.99   |
| 2   | L     | 435 | THR  | CA-C-N     | 5.61  | 131.01      | 122.65   |
| 2   | L     | 435 | THR  | C-N-CA     | 5.61  | 131.01      | 122.65   |
| 2   | I     | 894 | SER  | CA-C-N     | 5.61  | 130.17      | 121.26   |
| 2   | I     | 894 | SER  | C-N-CA     | 5.61  | 130.17      | 121.26   |
| 2   | L     | 844 | PRO  | N-CA-CB    | 5.60  | 106.06      | 102.92   |
| 2   | C     | 863 | CYS  | N-CA-C     | -5.60 | 98.69       | 107.93   |
| 2   | B     | 184 | PHE  | N-CA-CB    | -5.59 | 101.69      | 110.69   |
| 2   | I     | 899 | ASP  | CA-CB-CG   | 5.59  | 118.19      | 112.60   |
| 2   | J     | 543 | ARG  | NE-CZ-NH2  | 5.59  | 124.23      | 119.20   |
| 2   | L     | 543 | ARG  | NH1-CZ-NH2 | -5.59 | 112.04      | 119.30   |
| 2   | I     | 888 | ASN  | N-CA-CB    | 5.57  | 119.91      | 110.49   |
| 2   | I     | 907 | MET  | N-CA-C     | 5.56  | 120.22      | 113.38   |
| 2   | G     | 107 | LEU  | CB-CA-C    | -5.56 | 100.11      | 109.50   |
| 2   | J     | 286 | ASN  | CA-CB-CG   | 5.55  | 118.15      | 112.60   |
| 2   | C     | 708 | THR  | CA-CB-CG2  | 5.54  | 119.92      | 110.50   |
| 2   | I     | 737 | PRO  | N-CA-C     | 5.54  | 123.88      | 112.47   |
| 2   | K     | 667 | ARG  | N-CA-CB    | -5.54 | 101.70      | 111.39   |
| 2   | B     | 863 | CYS  | N-CA-C     | -5.53 | 98.81       | 107.93   |
| 2   | G     | 142 | THR  | CA-C-O     | -5.53 | 112.61      | 120.51   |
| 2   | E     | 177 | GLY  | CA-C-N     | 5.52  | 132.09      | 121.54   |
| 2   | E     | 177 | GLY  | C-N-CA     | 5.52  | 132.09      | 121.54   |
| 2   | F     | 148 | SER  | CA-C-N     | 5.52  | 131.91      | 121.97   |
| 2   | F     | 148 | SER  | C-N-CA     | 5.52  | 131.91      | 121.97   |
| 2   | I     | 109 | ARG  | NE-CZ-NH2  | 5.52  | 124.17      | 119.20   |
| 2   | E     | 890 | LEU  | CA-C-N     | 5.52  | 132.09      | 121.54   |
| 2   | E     | 890 | LEU  | C-N-CA     | 5.52  | 132.09      | 121.54   |
| 2   | L     | 599 | ARG  | N-CA-C     | -5.52 | 105.35      | 111.36   |
| 2   | I     | 447 | ASN  | OD1-CG-ND2 | -5.51 | 117.09      | 122.60   |
| 1   | 7     | 10  | ALA  | N-CA-C     | 5.51  | 121.99      | 109.81   |
| 2   | C     | 38  | TYR  | CB-CG-CD2  | -5.51 | 112.54      | 120.80   |
| 2   | J     | 543 | ARG  | NH1-CZ-NH2 | -5.51 | 112.14      | 119.30   |
| 2   | E     | 149 | VAL  | CB-CA-C    | -5.50 | 105.29      | 111.45   |
| 2   | C     | 431 | GLY  | CA-C-N     | 5.49  | 132.03      | 121.54   |
| 2   | C     | 431 | GLY  | C-N-CA     | 5.49  | 132.03      | 121.54   |
| 2   | C     | 864 | ASP  | CA-CB-CG   | 5.49  | 118.09      | 112.60   |
| 2   | F     | 376 | ARG  | NE-CZ-NH2  | 5.49  | 124.14      | 119.20   |
| 2   | F     | 606 | ARG  | NE-CZ-NH2  | 5.48  | 124.13      | 119.20   |
| 2   | K     | 899 | ASP  | CA-CB-CG   | 5.48  | 118.08      | 112.60   |
| 2   | H     | 235 | GLN  | OE1-CD-NE2 | -5.47 | 117.13      | 122.60   |
| 2   | B     | 138 | ASN  | N-CA-C     | 5.47  | 117.66      | 108.96   |
| 2   | I     | 668 | ASN  | OD1-CG-ND2 | -5.47 | 117.13      | 122.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | I     | 297 | LYS  | CB-CA-C    | 5.47  | 117.40      | 109.20   |
| 2   | F     | 92  | ARG  | NE-CZ-NH2  | 5.46  | 124.12      | 119.20   |
| 2   | E     | 607 | PHE  | CA-CB-CG   | 5.46  | 119.26      | 113.80   |
| 2   | B     | 84  | PHE  | CD1-CG-CD2 | -5.46 | 110.41      | 118.60   |
| 2   | B     | 728 | TRP  | CB-CA-C    | -5.46 | 104.15      | 113.04   |
| 2   | F     | 107 | LEU  | CB-CA-C    | -5.45 | 100.29      | 109.50   |
| 2   | I     | 267 | GLY  | CA-C-N     | 5.45  | 131.94      | 121.54   |
| 2   | I     | 267 | GLY  | C-N-CA     | 5.45  | 131.94      | 121.54   |
| 6   | S     | 76  | ARG  | NE-CZ-NH2  | 5.45  | 124.10      | 119.20   |
| 2   | C     | 946 | ASN  | CA-CB-CG   | 5.44  | 118.04      | 112.60   |
| 2   | H     | 800 | ARG  | NE-CZ-NH2  | 5.44  | 124.10      | 119.20   |
| 2   | C     | 943 | SER  | CB-CA-C    | -5.44 | 101.69      | 110.77   |
| 2   | E     | 198 | GLU  | N-CA-C     | 5.44  | 118.13      | 111.82   |
| 2   | C     | 417 | ASN  | N-CA-C     | 5.43  | 119.19      | 112.24   |
| 5   | O     | 192 | PHE  | N-CA-C     | 5.43  | 119.07      | 111.90   |
| 2   | A     | 708 | THR  | CA-CB-CG2  | 5.43  | 119.72      | 110.50   |
| 2   | K     | 807 | ASN  | N-CA-CB    | -5.43 | 104.00      | 112.41   |
| 2   | B     | 434 | GLU  | N-CA-C     | -5.42 | 100.77      | 109.39   |
| 2   | A     | 235 | GLN  | OE1-CD-NE2 | -5.42 | 117.18      | 122.60   |
| 2   | K     | 543 | ARG  | NH1-CZ-NH2 | -5.42 | 112.26      | 119.30   |
| 2   | L     | 773 | ILE  | N-CA-C     | 5.41  | 116.67      | 112.12   |
| 2   | G     | 109 | ARG  | NE-CZ-NH2  | 5.41  | 124.07      | 119.20   |
| 2   | I     | 357 | ASP  | N-CA-CB    | -5.41 | 102.97      | 110.65   |
| 2   | K     | 179 | ALA  | CA-C-N     | -5.41 | 115.26      | 122.72   |
| 2   | K     | 179 | ALA  | C-N-CA     | -5.41 | 115.26      | 122.72   |
| 2   | E     | 634 | ASP  | CA-CB-CG   | 5.40  | 118.00      | 112.60   |
| 1   | 4     | 16  | ARG  | NE-CZ-NH2  | 5.40  | 124.06      | 119.20   |
| 2   | C     | 438 | ASP  | CA-CB-CG   | 5.39  | 117.99      | 112.60   |
| 1   | 8     | 18  | PHE  | N-CA-CB    | -5.39 | 104.15      | 110.35   |
| 1   | 7     | 18  | PHE  | CA-CB-CG   | 5.39  | 119.19      | 113.80   |
| 2   | A     | 773 | ILE  | N-CA-C     | 5.38  | 116.04      | 110.82   |
| 2   | A     | 273 | GLU  | N-CA-C     | 5.38  | 122.26      | 110.80   |
| 2   | B     | 303 | GLU  | N-CA-C     | 5.38  | 117.81      | 110.55   |
| 2   | I     | 534 | HIS  | CB-CG-CD2  | -5.38 | 124.21      | 131.20   |
| 2   | J     | 374 | ARG  | NE-CZ-NH2  | 5.38  | 124.04      | 119.20   |
| 2   | B     | 820 | HIS  | CB-CG-CD2  | -5.37 | 124.22      | 131.20   |
| 2   | B     | 184 | PHE  | CD1-CG-CD2 | -5.37 | 110.55      | 118.60   |
| 2   | C     | 184 | PHE  | CD1-CG-CD2 | -5.36 | 110.57      | 118.60   |
| 2   | I     | 811 | TYR  | N-CA-C     | 5.36  | 117.94      | 109.96   |
| 2   | B     | 239 | LYS  | CB-CA-C    | 5.35  | 118.58      | 109.53   |
| 2   | E     | 924 | ARG  | NE-CZ-NH2  | 5.35  | 124.02      | 119.20   |
| 2   | G     | 137 | ALA  | CA-C-N     | -5.35 | 113.21      | 122.14   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | G     | 137 | ALA  | C-N-CA     | -5.35 | 113.21      | 122.14   |
| 2   | E     | 146 | PRO  | N-CA-C     | -5.34 | 101.47      | 112.47   |
| 2   | F     | 139 | GLU  | CA-C-O     | 5.34  | 127.00      | 120.92   |
| 2   | G     | 855 | SER  | N-CA-C     | 5.33  | 118.13      | 109.06   |
| 3   | M     | 281 | ASP  | CA-CB-CG   | 5.33  | 117.93      | 112.60   |
| 2   | K     | 285 | VAL  | N-CA-CB    | -5.33 | 103.36      | 111.57   |
| 2   | L     | 432 | ALA  | N-CA-C     | -5.33 | 101.55      | 109.11   |
| 2   | J     | 188 | THR  | O-C-N      | -5.32 | 117.26      | 123.27   |
| 2   | G     | 136 | THR  | N-CA-C     | 5.32  | 117.21      | 109.71   |
| 2   | D     | 376 | ARG  | NE-CZ-NH2  | 5.31  | 123.98      | 119.20   |
| 2   | E     | 433 | GLU  | N-CA-C     | -5.31 | 101.22      | 109.72   |
| 2   | C     | 435 | THR  | N-CA-C     | 5.31  | 118.25      | 108.58   |
| 2   | B     | 642 | ASP  | N-CA-C     | -5.31 | 102.19      | 110.10   |
| 2   | K     | 180 | THR  | N-CA-C     | 5.31  | 117.89      | 109.24   |
| 2   | C     | 338 | ASN  | N-CA-CB    | -5.31 | 103.65      | 111.51   |
| 5   | P     | 48  | ARG  | NE-CZ-NH2  | 5.30  | 123.97      | 119.20   |
| 2   | J     | 334 | ASN  | OD1-CG-ND2 | -5.29 | 117.31      | 122.60   |
| 2   | B     | 417 | ASN  | N-CA-C     | 5.29  | 119.02      | 112.24   |
| 2   | K     | 374 | ARG  | NE-CZ-NH2  | 5.29  | 123.96      | 119.20   |
| 2   | K     | 924 | ARG  | NE-CZ-NH2  | 5.29  | 123.96      | 119.20   |
| 2   | G     | 409 | PHE  | CA-C-N     | 5.29  | 125.22      | 119.78   |
| 2   | G     | 409 | PHE  | C-N-CA     | 5.29  | 125.22      | 119.78   |
| 2   | I     | 510 | LEU  | N-CA-C     | -5.28 | 102.47      | 110.28   |
| 2   | H     | 285 | VAL  | CA-CB-CG1  | 5.28  | 119.38      | 110.40   |
| 2   | I     | 7   | MET  | N-CA-C     | 5.28  | 120.85      | 113.57   |
| 2   | L     | 514 | TYR  | N-CA-CB    | -5.28 | 102.68      | 110.49   |
| 1   | 7     | 6   | PHE  | CA-CB-CG   | 5.28  | 119.08      | 113.80   |
| 2   | I     | 924 | ARG  | NE-CZ-NH2  | 5.27  | 123.95      | 119.20   |
| 2   | K     | 599 | ARG  | N-CA-C     | -5.27 | 105.20      | 111.69   |
| 2   | G     | 776 | GLN  | N-CA-C     | 5.27  | 118.66      | 111.39   |
| 2   | I     | 107 | LEU  | CB-CA-C    | -5.27 | 100.60      | 109.50   |
| 3   | M     | 105 | ARG  | NE-CZ-NH2  | 5.27  | 123.94      | 119.20   |
| 2   | G     | 7   | MET  | N-CA-C     | 5.27  | 120.84      | 113.57   |
| 2   | C     | 303 | GLU  | N-CA-C     | 5.26  | 117.66      | 110.55   |
| 2   | G     | 599 | ARG  | N-CA-C     | -5.26 | 104.98      | 111.40   |
| 2   | G     | 922 | VAL  | N-CA-C     | 5.26  | 116.16      | 108.53   |
| 6   | S     | 60  | ASP  | CA-CB-CG   | 5.26  | 117.86      | 112.60   |
| 2   | F     | 303 | GLU  | N-CA-C     | 5.25  | 116.87      | 110.41   |
| 2   | L     | 260 | PRO  | CA-C-N     | 5.25  | 136.49      | 122.78   |
| 2   | L     | 260 | PRO  | C-N-CA     | 5.25  | 136.49      | 122.78   |
| 2   | F     | 140 | LYS  | CA-CB-CG   | 5.25  | 124.59      | 114.10   |
| 2   | B     | 407 | TYR  | N-CA-C     | 5.24  | 117.62      | 108.76   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | C     | 645 | SER  | N-CA-C     | 5.24  | 117.91      | 110.10   |
| 2   | I     | 273 | GLU  | N-CA-C     | 5.24  | 119.64      | 112.88   |
| 2   | D     | 697 | VAL  | CA-CB-CG1  | 5.24  | 119.31      | 110.40   |
| 2   | L     | 332 | TYR  | CD1-CG-CD2 | -5.24 | 110.25      | 118.10   |
| 2   | K     | 37  | THR  | CA-C-N     | 5.24  | 131.12      | 121.70   |
| 2   | K     | 37  | THR  | C-N-CA     | 5.24  | 131.12      | 121.70   |
| 2   | G     | 564 | PHE  | N-CA-C     | 5.23  | 116.98      | 111.28   |
| 2   | C     | 52  | PRO  | N-CA-C     | 5.22  | 120.47      | 114.20   |
| 2   | G     | 510 | LEU  | N-CA-C     | -5.22 | 102.55      | 110.28   |
| 2   | L     | 616 | PHE  | CA-CB-CG   | 5.22  | 119.02      | 113.80   |
| 2   | G     | 249 | ASP  | N-CA-C     | 5.22  | 117.61      | 109.52   |
| 2   | L     | 374 | ARG  | NE-CZ-NH2  | 5.22  | 123.90      | 119.20   |
| 2   | I     | 146 | PRO  | CB-CA-C    | 5.22  | 118.15      | 111.21   |
| 2   | A     | 520 | ARG  | NE-CZ-NH2  | 5.20  | 123.88      | 119.20   |
| 2   | B     | 930 | ARG  | CB-CA-C    | 5.20  | 120.25      | 110.63   |
| 3   | M     | 449 | ASP  | CA-CB-CG   | 5.20  | 117.80      | 112.60   |
| 2   | B     | 43  | ASN  | CA-CB-CG   | 5.20  | 117.80      | 112.60   |
| 2   | B     | 855 | SER  | N-CA-CB    | -5.20 | 101.86      | 111.52   |
| 2   | C     | 896 | HIS  | CB-CG-CD2  | -5.20 | 124.44      | 131.20   |
| 2   | J     | 888 | ASN  | CA-C-N     | 5.19  | 131.21      | 123.05   |
| 2   | J     | 888 | ASN  | C-N-CA     | 5.19  | 131.21      | 123.05   |
| 2   | D     | 606 | ARG  | NE-CZ-NH2  | 5.19  | 123.87      | 119.20   |
| 2   | B     | 899 | ASP  | CA-CB-CG   | 5.19  | 117.79      | 112.60   |
| 2   | C     | 429 | GLN  | OE1-CD-NE2 | -5.19 | 117.41      | 122.60   |
| 2   | G     | 924 | ARG  | NE-CZ-NH2  | 5.19  | 123.87      | 119.20   |
| 2   | H     | 374 | ARG  | NE-CZ-NH2  | 5.18  | 123.87      | 119.20   |
| 2   | B     | 143 | GLY  | CA-C-N     | 5.18  | 125.73      | 119.98   |
| 2   | B     | 143 | GLY  | C-N-CA     | 5.18  | 125.73      | 119.98   |
| 2   | D     | 334 | ASN  | OD1-CG-ND2 | -5.18 | 117.42      | 122.60   |
| 2   | G     | 263 | THR  | CA-C-N     | 5.18  | 125.71      | 120.38   |
| 2   | G     | 263 | THR  | C-N-CA     | 5.18  | 125.71      | 120.38   |
| 2   | J     | 926 | HIS  | CB-CG-CD2  | -5.18 | 124.47      | 131.20   |
| 2   | K     | 617 | PHE  | CB-CG-CD2  | -5.18 | 111.90      | 120.70   |
| 2   | A     | 744 | ARG  | NE-CZ-NH2  | 5.17  | 123.86      | 119.20   |
| 5   | P     | 168 | TYR  | CA-CB-CG   | 5.17  | 123.21      | 113.90   |
| 2   | K     | 942 | PHE  | N-CA-C     | -5.17 | 104.30      | 111.28   |
| 2   | A     | 756 | CYS  | N-CA-CB    | -5.17 | 103.50      | 111.46   |
| 2   | F     | 140 | LYS  | CA-C-N     | -5.17 | 111.67      | 121.54   |
| 2   | F     | 140 | LYS  | C-N-CA     | -5.17 | 111.67      | 121.54   |
| 3   | M     | 101 | ASP  | CA-CB-CG   | -5.17 | 107.43      | 112.60   |
| 2   | B     | 271 | GLN  | N-CA-CB    | -5.16 | 101.77      | 110.49   |
| 2   | I     | 67  | ARG  | NE-CZ-NH2  | 5.15  | 123.84      | 119.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | E     | 564 | PHE  | N-CA-C     | 5.15  | 116.90      | 111.28   |
| 2   | F     | 543 | ARG  | NE-CZ-NH2  | 5.15  | 123.84      | 119.20   |
| 2   | I     | 887 | GLN  | CA-C-N     | 5.15  | 131.38      | 121.54   |
| 2   | I     | 887 | GLN  | C-N-CA     | 5.15  | 131.38      | 121.54   |
| 2   | L     | 202 | GLU  | CB-CA-C    | -5.15 | 101.47      | 109.61   |
| 2   | J     | 673 | ARG  | NE-CZ-NH2  | 5.15  | 123.84      | 119.20   |
| 2   | K     | 188 | THR  | N-CA-C     | -5.15 | 100.12      | 108.52   |
| 2   | B     | 18  | GLN  | N-CA-C     | 5.14  | 117.34      | 110.35   |
| 2   | K     | 258 | ASP  | CA-CB-CG   | 5.14  | 117.74      | 112.60   |
| 2   | C     | 374 | ARG  | NE-CZ-NH2  | 5.14  | 123.83      | 119.20   |
| 2   | C     | 941 | PRO  | N-CA-CB    | 5.14  | 108.22      | 103.39   |
| 2   | K     | 830 | ALA  | N-CA-CB    | -5.14 | 105.71      | 111.10   |
| 2   | C     | 487 | ALA  | N-CA-C     | 5.13  | 117.61      | 111.71   |
| 2   | C     | 274 | TYR  | N-CA-C     | -5.13 | 102.86      | 110.46   |
| 2   | G     | 374 | ARG  | NE-CZ-NH2  | 5.13  | 123.82      | 119.20   |
| 2   | I     | 791 | PHE  | N-CA-C     | 5.13  | 116.56      | 110.97   |
| 1   | 8     | 22  | TRP  | N-CA-C     | 5.13  | 117.55      | 109.39   |
| 2   | A     | 645 | SER  | N-CA-C     | 5.13  | 117.78      | 110.24   |
| 2   | I     | 943 | SER  | CB-CA-C    | -5.13 | 101.68      | 109.89   |
| 2   | K     | 434 | GLU  | CA-C-N     | 5.13  | 131.33      | 121.54   |
| 2   | K     | 434 | GLU  | C-N-CA     | 5.13  | 131.33      | 121.54   |
| 2   | B     | 207 | TYR  | CA-C-N     | 5.12  | 125.72      | 122.18   |
| 2   | B     | 207 | TYR  | C-N-CA     | 5.12  | 125.72      | 122.18   |
| 2   | B     | 943 | SER  | N-CA-C     | 5.12  | 117.14      | 110.43   |
| 2   | C     | 744 | ARG  | NE-CZ-NH2  | 5.12  | 123.80      | 119.20   |
| 2   | L     | 663 | SER  | CA-C-N     | 5.11  | 127.78      | 123.33   |
| 2   | L     | 663 | SER  | C-N-CA     | 5.11  | 127.78      | 123.33   |
| 1   | 3     | 17  | PRO  | CA-C-N     | 5.11  | 131.30      | 121.54   |
| 1   | 3     | 17  | PRO  | C-N-CA     | 5.11  | 131.30      | 121.54   |
| 2   | L     | 891 | TYR  | CA-C-N     | 5.11  | 128.80      | 121.50   |
| 2   | L     | 891 | TYR  | C-N-CA     | 5.11  | 128.80      | 121.50   |
| 2   | D     | 520 | ARG  | NE-CZ-NH2  | 5.10  | 123.79      | 119.20   |
| 2   | G     | 201 | GLN  | CB-CA-C    | -5.10 | 103.15      | 111.06   |
| 2   | D     | 800 | ARG  | NE-CZ-NH2  | 5.10  | 123.79      | 119.20   |
| 6   | S     | 101 | LEU  | N-CA-C     | 5.10  | 118.43      | 110.32   |
| 2   | C     | 926 | HIS  | CB-CG-CD2  | -5.09 | 124.58      | 131.20   |
| 2   | G     | 83  | ARG  | NE-CZ-NH2  | 5.09  | 123.78      | 119.20   |
| 2   | L     | 667 | ARG  | N-CA-CB    | -5.09 | 102.47      | 111.39   |
| 2   | K     | 303 | GLU  | N-CA-C     | 5.09  | 116.67      | 110.41   |
| 2   | L     | 943 | SER  | O-C-N      | -5.09 | 115.96      | 122.83   |
| 2   | E     | 348 | GLN  | OE1-CD-NE2 | -5.09 | 117.51      | 122.60   |
| 2   | H     | 263 | THR  | CA-C-N     | 5.09  | 125.62      | 120.38   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | H     | 263 | THR  | C-N-CA     | 5.09  | 125.62      | 120.38   |
| 2   | H     | 611 | ASN  | CA-CB-CG   | 5.08  | 117.68      | 112.60   |
| 2   | E     | 432 | ALA  | CA-C-N     | 5.07  | 130.78      | 122.81   |
| 2   | E     | 432 | ALA  | C-N-CA     | 5.07  | 130.78      | 122.81   |
| 2   | H     | 835 | GLN  | OE1-CD-NE2 | -5.07 | 117.53      | 122.60   |
| 2   | I     | 926 | HIS  | CB-CG-CD2  | -5.07 | 124.61      | 131.20   |
| 5   | O     | 212 | PHE  | CA-CB-CG   | 5.07  | 118.87      | 113.80   |
| 1   | 5     | 22  | TRP  | N-CA-C     | 5.07  | 116.31      | 107.49   |
| 2   | L     | 78  | TYR  | CA-CB-CG   | 5.07  | 123.02      | 113.90   |
| 2   | K     | 663 | SER  | CA-C-N     | 5.07  | 127.74      | 123.33   |
| 2   | K     | 663 | SER  | C-N-CA     | 5.07  | 127.74      | 123.33   |
| 1   | 3     | 19  | MET  | N-CA-C     | 5.06  | 121.58      | 110.80   |
| 2   | C     | 90  | ASP  | N-CA-C     | 5.06  | 118.23      | 111.75   |
| 2   | A     | 924 | ARG  | NE-CZ-NH2  | 5.06  | 123.75      | 119.20   |
| 2   | A     | 632 | ARG  | NE-CZ-NH2  | 5.06  | 123.75      | 119.20   |
| 2   | C     | 866 | VAL  | CA-CB-CG1  | 5.05  | 118.99      | 110.40   |
| 2   | B     | 924 | ARG  | NE-CZ-NH2  | 5.05  | 123.75      | 119.20   |
| 2   | C     | 457 | MET  | CB-CA-C    | 5.05  | 118.48      | 109.65   |
| 2   | H     | 896 | HIS  | N-CA-C     | 5.04  | 117.54      | 110.23   |
| 2   | D     | 537 | ASN  | CA-CB-CG   | 5.04  | 117.64      | 112.60   |
| 5   | P     | 30  | ARG  | NE-CZ-NH2  | 5.04  | 123.73      | 119.20   |
| 2   | G     | 535 | HIS  | CB-CG-CD2  | -5.03 | 124.66      | 131.20   |
| 2   | I     | 892 | ALA  | CA-C-N     | 5.03  | 131.16      | 121.54   |
| 2   | I     | 892 | ALA  | C-N-CA     | 5.03  | 131.16      | 121.54   |
| 5   | O     | 224 | ASP  | CA-CB-CG   | 5.03  | 117.63      | 112.60   |
| 2   | C     | 336 | THR  | N-CA-C     | 5.03  | 116.45      | 111.07   |
| 2   | I     | 311 | GLN  | OE1-CD-NE2 | -5.03 | 117.57      | 122.60   |
| 5   | P     | 212 | PHE  | CA-CB-CG   | 5.03  | 118.83      | 113.80   |
| 2   | E     | 800 | ARG  | NE-CZ-NH2  | 5.03  | 123.72      | 119.20   |
| 2   | C     | 114 | LYS  | CA-C-N     | 5.02  | 126.12      | 119.84   |
| 2   | C     | 114 | LYS  | C-N-CA     | 5.02  | 126.12      | 119.84   |
| 2   | E     | 744 | ARG  | NE-CZ-NH2  | 5.02  | 123.72      | 119.20   |
| 2   | I     | 893 | ASN  | CA-CB-CG   | 5.02  | 117.62      | 112.60   |
| 2   | I     | 200 | TRP  | CB-CG-CD2  | -5.02 | 119.77      | 126.80   |
| 2   | C     | 9   | GLN  | OE1-CD-NE2 | -5.02 | 117.58      | 122.60   |
| 2   | C     | 266 | THR  | CB-CA-C    | 5.02  | 117.86      | 110.14   |
| 2   | C     | 756 | CYS  | N-CA-CB    | -5.01 | 103.74      | 111.46   |
| 2   | I     | 210 | ARG  | NE-CZ-NH2  | 5.01  | 123.71      | 119.20   |
| 2   | J     | 941 | PRO  | N-CA-CB    | 5.01  | 108.52      | 103.25   |
| 2   | B     | 708 | THR  | CA-CB-CG2  | 5.01  | 119.02      | 110.50   |
| 1   | 1     | 22  | TRP  | N-CA-C     | 5.01  | 118.93      | 111.87   |
| 2   | H     | 83  | ARG  | NE-CZ-NH2  | 5.01  | 123.71      | 119.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | E     | 407 | TYR  | CA-C-N     | 5.01  | 130.45      | 122.74   |
| 2   | E     | 407 | TYR  | C-N-CA     | 5.01  | 130.45      | 122.74   |
| 2   | F     | 738 | ASN  | CA-C-N     | 5.01  | 130.74      | 122.33   |
| 2   | F     | 738 | ASN  | C-N-CA     | 5.01  | 130.74      | 122.33   |
| 2   | H     | 776 | GLN  | OE1-CD-NE2 | -5.01 | 117.59      | 122.60   |

There are no chirality outliers.

All (149) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | 3     | 19  | MET  | Peptide   |
| 2   | A     | 140 | LYS  | Peptide   |
| 2   | A     | 407 | TYR  | Sidechain |
| 2   | A     | 433 | GLU  | Peptide   |
| 2   | A     | 80  | TYR  | Sidechain |
| 2   | B     | 184 | PHE  | Sidechain |
| 2   | B     | 281 | TYR  | Sidechain |
| 2   | B     | 38  | TYR  | Sidechain |
| 2   | B     | 407 | TYR  | Sidechain |
| 2   | B     | 420 | TYR  | Sidechain |
| 2   | B     | 46  | ARG  | Sidechain |
| 2   | B     | 498 | TYR  | Sidechain |
| 2   | B     | 541 | ARG  | Sidechain |
| 2   | B     | 599 | ARG  | Sidechain |
| 2   | B     | 667 | ARG  | Sidechain |
| 2   | B     | 695 | TYR  | Sidechain |
| 2   | B     | 84  | PHE  | Sidechain |
| 2   | B     | 869 | ARG  | Sidechain |
| 2   | C     | 184 | PHE  | Sidechain |
| 2   | C     | 274 | TYR  | Sidechain |
| 2   | C     | 281 | TYR  | Sidechain |
| 2   | C     | 332 | TYR  | Sidechain |
| 2   | C     | 38  | TYR  | Sidechain |
| 2   | C     | 407 | TYR  | Sidechain |
| 2   | C     | 695 | TYR  | Sidechain |
| 2   | C     | 698 | TYR  | Sidechain |
| 2   | C     | 704 | TYR  | Sidechain |
| 2   | C     | 8   | PRO  | Mainchain |
| 2   | C     | 80  | TYR  | Sidechain |
| 2   | C     | 83  | ARG  | Sidechain |
| 2   | C     | 84  | PHE  | Sidechain |
| 2   | C     | 869 | ARG  | Sidechain |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 2   | D     | 109 | ARG  | Sidechain         |
| 2   | D     | 116 | TYR  | Sidechain         |
| 2   | D     | 12  | TYR  | Sidechain         |
| 2   | D     | 407 | TYR  | Sidechain         |
| 2   | D     | 498 | TYR  | Sidechain         |
| 2   | D     | 599 | ARG  | Sidechain         |
| 2   | D     | 613 | TYR  | Sidechain         |
| 2   | D     | 695 | TYR  | Sidechain         |
| 2   | D     | 865 | ARG  | Sidechain         |
| 2   | E     | 109 | ARG  | Sidechain         |
| 2   | E     | 175 | GLU  | Peptide           |
| 2   | E     | 176 | GLU  | Mainchain,Peptide |
| 2   | E     | 202 | GLU  | Peptide           |
| 2   | E     | 274 | TYR  | Sidechain         |
| 2   | E     | 320 | TYR  | Sidechain         |
| 2   | E     | 377 | TYR  | Sidechain         |
| 2   | E     | 407 | TYR  | Sidechain         |
| 2   | E     | 420 | TYR  | Sidechain         |
| 2   | E     | 433 | GLU  | Mainchain         |
| 2   | E     | 500 | TYR  | Sidechain         |
| 2   | E     | 784 | TYR  | Sidechain         |
| 2   | E     | 869 | ARG  | Sidechain         |
| 2   | F     | 109 | ARG  | Sidechain         |
| 2   | F     | 116 | TYR  | Sidechain         |
| 2   | F     | 136 | THR  | Mainchain,Peptide |
| 2   | F     | 139 | GLU  | Peptide           |
| 2   | F     | 265 | PRO  | Peptide           |
| 2   | F     | 268 | SER  | Peptide           |
| 2   | F     | 323 | PHE  | Sidechain         |
| 2   | F     | 332 | TYR  | Sidechain         |
| 2   | F     | 407 | TYR  | Sidechain         |
| 2   | F     | 500 | TYR  | Sidechain         |
| 2   | F     | 541 | ARG  | Sidechain         |
| 2   | F     | 555 | PHE  | Sidechain         |
| 2   | F     | 599 | ARG  | Sidechain         |
| 2   | F     | 695 | TYR  | Sidechain         |
| 2   | F     | 737 | PRO  | Peptide           |
| 2   | F     | 869 | ARG  | Sidechain         |
| 2   | G     | 109 | ARG  | Sidechain         |
| 2   | G     | 121 | TYR  | Sidechain         |
| 2   | G     | 137 | ALA  | Mainchain         |
| 2   | G     | 141 | GLN  | Peptide           |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | G     | 388 | TYR  | Sidechain |
| 2   | G     | 407 | TYR  | Sidechain |
| 2   | G     | 455 | TYR  | Sidechain |
| 2   | G     | 599 | ARG  | Sidechain |
| 2   | G     | 63  | ARG  | Sidechain |
| 2   | G     | 643 | TYR  | Sidechain |
| 2   | G     | 67  | ARG  | Sidechain |
| 2   | G     | 695 | TYR  | Sidechain |
| 2   | G     | 84  | PHE  | Sidechain |
| 2   | G     | 869 | ARG  | Sidechain |
| 2   | G     | 891 | TYR  | Sidechain |
| 2   | G     | 896 | HIS  | Sidechain |
| 2   | H     | 109 | ARG  | Sidechain |
| 2   | H     | 320 | TYR  | Sidechain |
| 2   | H     | 374 | ARG  | Sidechain |
| 2   | H     | 407 | TYR  | Sidechain |
| 2   | H     | 599 | ARG  | Sidechain |
| 2   | H     | 706 | ASP  | Peptide   |
| 2   | H     | 78  | TYR  | Sidechain |
| 2   | H     | 869 | ARG  | Sidechain |
| 2   | I     | 109 | ARG  | Sidechain |
| 2   | I     | 332 | TYR  | Sidechain |
| 2   | I     | 407 | TYR  | Sidechain |
| 2   | I     | 599 | ARG  | Sidechain |
| 2   | I     | 606 | ARG  | Sidechain |
| 2   | I     | 677 | PHE  | Sidechain |
| 2   | I     | 78  | TYR  | Sidechain |
| 2   | I     | 84  | PHE  | Sidechain |
| 2   | J     | 109 | ARG  | Sidechain |
| 2   | J     | 116 | TYR  | Sidechain |
| 2   | J     | 121 | TYR  | Sidechain |
| 2   | J     | 38  | TYR  | Sidechain |
| 2   | J     | 46  | ARG  | Sidechain |
| 2   | J     | 498 | TYR  | Sidechain |
| 2   | J     | 543 | ARG  | Sidechain |
| 2   | J     | 673 | ARG  | Sidechain |
| 2   | J     | 688 | LEU  | Peptide   |
| 2   | K     | 109 | ARG  | Sidechain |
| 2   | K     | 38  | TYR  | Sidechain |
| 2   | K     | 430 | ASP  | Peptide   |
| 2   | K     | 46  | ARG  | Sidechain |
| 2   | K     | 514 | TYR  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | K     | 599 | ARG  | Sidechain |
| 2   | K     | 617 | PHE  | Sidechain |
| 2   | K     | 67  | ARG  | Sidechain |
| 2   | K     | 7   | MET  | Peptide   |
| 2   | K     | 744 | ARG  | Sidechain |
| 2   | K     | 891 | TYR  | Sidechain |
| 2   | L     | 109 | ARG  | Sidechain |
| 2   | L     | 116 | TYR  | Sidechain |
| 2   | L     | 320 | TYR  | Sidechain |
| 2   | L     | 332 | TYR  | Sidechain |
| 2   | L     | 38  | TYR  | Sidechain |
| 2   | L     | 46  | ARG  | Sidechain |
| 2   | L     | 514 | TYR  | Sidechain |
| 2   | L     | 599 | ARG  | Sidechain |
| 2   | L     | 60  | ARG  | Sidechain |
| 2   | L     | 617 | PHE  | Sidechain |
| 2   | L     | 67  | ARG  | Sidechain |
| 2   | L     | 698 | TYR  | Sidechain |
| 2   | L     | 710 | TYR  | Sidechain |
| 2   | L     | 78  | TYR  | Sidechain |
| 2   | L     | 792 | PHE  | Sidechain |
| 2   | L     | 83  | ARG  | Sidechain |
| 2   | L     | 891 | TYR  | Sidechain |
| 3   | M     | 386 | TYR  | Sidechain |
| 3   | M     | 396 | PRO  | Peptide   |
| 3   | M     | 484 | ARG  | Sidechain |
| 3   | M     | 497 | ARG  | Sidechain |
| 4   | N     | 93  | TYR  | Sidechain |
| 5   | O     | 27  | TYR  | Sidechain |
| 5   | O     | 30  | ARG  | Sidechain |
| 5   | O     | 72  | ARG  | Sidechain |

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1     | 177   | 163      | 162      | 2       | 0            |
| 1   | 2     | 113   | 103      | 102      | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 1   | 3     | 168    | 157      | 156      | 2       | 0            |
| 1   | 4     | 91     | 81       | 80       | 2       | 0            |
| 1   | 5     | 202    | 191      | 191      | 3       | 0            |
| 1   | 6     | 161    | 148      | 147      | 1       | 0            |
| 1   | 7     | 211    | 204      | 203      | 1       | 0            |
| 1   | 8     | 140    | 131      | 129      | 1       | 0            |
| 2   | A     | 7491   | 7148     | 7145     | 11      | 0            |
| 2   | B     | 7491   | 7148     | 7145     | 22      | 0            |
| 2   | C     | 7491   | 7149     | 7146     | 21      | 0            |
| 2   | D     | 7491   | 7149     | 7146     | 12      | 0            |
| 2   | E     | 7491   | 7148     | 7145     | 33      | 0            |
| 2   | F     | 7491   | 7148     | 7145     | 37      | 0            |
| 2   | G     | 7491   | 7149     | 7146     | 26      | 0            |
| 2   | H     | 7491   | 7148     | 7145     | 4       | 0            |
| 2   | I     | 7491   | 7148     | 7145     | 39      | 0            |
| 2   | J     | 7491   | 7148     | 7145     | 12      | 0            |
| 2   | K     | 7491   | 7148     | 7145     | 26      | 0            |
| 2   | L     | 7475   | 7129     | 7129     | 50      | 0            |
| 3   | M     | 3794   | 3715     | 3712     | 2       | 0            |
| 4   | N     | 2176   | 2170     | 2169     | 2       | 0            |
| 5   | O     | 1377   | 1329     | 1327     | 4       | 0            |
| 5   | P     | 1389   | 1338     | 1336     | 4       | 0            |
| 6   | Q     | 302    | 317      | 317      | 0       | 0            |
| 6   | R     | 285    | 294      | 293      | 0       | 0            |
| 6   | S     | 504    | 513      | 511      | 3       | 0            |
| 6   | T     | 255    | 261      | 260      | 0       | 0            |
| All | All   | 101221 | 96875    | 96822    | 281     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (281) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:F:734:LEU:HB2  | 2:F:737:PRO:CG  | 2.12                     | 0.79              |
| 2:F:495:THR:HA   | 2:F:500:TYR:CD2 | 2.20                     | 0.77              |
| 2:B:191:PRO:HG3  | 2:B:281:TYR:CD2 | 2.22                     | 0.73              |
| 2:F:495:THR:HG22 | 2:F:500:TYR:CE2 | 2.26                     | 0.71              |
| 2:I:736:THR:H    | 2:I:737:PRO:CD  | 2.06                     | 0.69              |
| 2:G:142:THR:HG23 | 2:G:145:GLN:C   | 2.18                     | 0.69              |
| 2:G:142:THR:HG22 | 2:G:143:GLY:H   | 1.60                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:734:LEU:HB2  | 2:F:737:PRO:CD   | 2.26                     | 0.65              |
| 2:C:191:PRO:HG3  | 2:C:281:TYR:CD2  | 2.30                     | 0.64              |
| 2:E:200:TRP:HE1  | 2:E:412:ASN:HA   | 1.61                     | 0.64              |
| 2:C:166:GLU:HB3  | 2:C:184:PHE:CD2  | 2.32                     | 0.64              |
| 2:I:84:PHE:CD2   | 2:I:612:LEU:HB2  | 2.33                     | 0.64              |
| 2:F:724:SER:HB2  | 2:L:69:VAL:HG22  | 1.78                     | 0.64              |
| 2:I:736:THR:H    | 2:I:737:PRO:HD3  | 1.62                     | 0.64              |
| 2:F:734:LEU:HB2  | 2:F:737:PRO:HG2  | 1.78                     | 0.63              |
| 2:G:84:PHE:CD2   | 2:G:612:LEU:HB2  | 2.33                     | 0.63              |
| 2:I:936:VAL:HG23 | 5:P:40:MET:HE3   | 1.79                     | 0.63              |
| 2:B:267:GLY:C    | 2:B:269:GLY:H    | 2.07                     | 0.62              |
| 2:G:84:PHE:CE2   | 2:G:612:LEU:HB2  | 2.34                     | 0.62              |
| 2:C:684:GLU:HG2  | 2:C:698:TYR:CE2  | 2.35                     | 0.62              |
| 2:E:495:THR:HA   | 2:E:500:TYR:CD2  | 2.34                     | 0.62              |
| 2:J:113:PHE:CZ   | 2:J:115:PRO:HG3  | 2.35                     | 0.61              |
| 2:F:734:LEU:HB2  | 2:F:737:PRO:HD2  | 1.81                     | 0.61              |
| 4:N:188:THR:HA   | 4:N:196:VAL:HG22 | 1.82                     | 0.60              |
| 2:L:83:ARG:HD2   | 2:L:577:THR:HG23 | 1.84                     | 0.60              |
| 2:K:512:ASP:HB3  | 2:K:514:TYR:CD1  | 2.37                     | 0.59              |
| 2:L:512:ASP:HB3  | 2:L:514:TYR:CD1  | 2.38                     | 0.59              |
| 2:L:332:TYR:CE1  | 2:L:583:ARG:HG2  | 2.38                     | 0.59              |
| 2:F:734:LEU:CB   | 2:F:737:PRO:HG2  | 2.33                     | 0.59              |
| 2:G:367:LEU:HA   | 2:G:643:TYR:CD2  | 2.38                     | 0.59              |
| 2:C:191:PRO:HG3  | 2:C:281:TYR:CE2  | 2.37                     | 0.58              |
| 2:I:84:PHE:CE2   | 2:I:612:LEU:HB2  | 2.38                     | 0.58              |
| 2:I:264:PRO:HG2  | 2:I:266:THR:HG22 | 1.86                     | 0.57              |
| 2:F:107:LEU:HD23 | 2:F:605:VAL:HG22 | 1.86                     | 0.57              |
| 2:F:734:LEU:CD1  | 2:F:737:PRO:HG2  | 2.34                     | 0.57              |
| 2:E:320:TYR:CE2  | 2:E:541:ARG:HG2  | 2.39                     | 0.57              |
| 2:G:142:THR:HG22 | 2:G:143:GLY:N    | 2.20                     | 0.57              |
| 2:L:320:TYR:CE2  | 2:L:541:ARG:HG2  | 2.40                     | 0.57              |
| 2:D:457:MET:HE1  | 2:E:457:MET:HG3  | 1.84                     | 0.57              |
| 2:C:426:LYS:HG2  | 2:C:429:GLN:HB2  | 1.86                     | 0.56              |
| 2:E:893:ASN:HA   | 2:I:346:ALA:HB1  | 1.85                     | 0.56              |
| 2:L:261:GLY:HA3  | 2:L:270:GLN:HB2  | 1.87                     | 0.56              |
| 2:E:200:TRP:CZ3  | 2:F:310:THR:HA   | 2.41                     | 0.56              |
| 2:L:885:LEU:O    | 2:L:891:TYR:CD2  | 2.58                     | 0.56              |
| 2:E:176:GLU:O    | 2:E:177:GLY:C    | 2.49                     | 0.56              |
| 2:K:514:TYR:CD2  | 2:K:844:PRO:HG3  | 2.41                     | 0.55              |
| 2:F:734:LEU:HD12 | 2:F:737:PRO:HG2  | 1.88                     | 0.55              |
| 2:K:457:MET:HE2  | 2:L:457:MET:HE2  | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:4:15:THR:HG22  | 1:4:16:ARG:H     | 1.71                     | 0.55              |
| 2:L:113:PHE:CZ   | 2:L:115:PRO:HG3  | 2.41                     | 0.55              |
| 4:N:193:LEU:O    | 4:N:196:VAL:HG23 | 2.06                     | 0.55              |
| 2:L:710:TYR:CD1  | 2:L:711:LEU:HG   | 2.42                     | 0.55              |
| 1:5:10:ALA:HB1   | 1:5:11:PRO:HD2   | 1.88                     | 0.55              |
| 2:B:166:GLU:HB3  | 2:B:184:PHE:CD2  | 2.42                     | 0.55              |
| 2:B:174:GLU:HA   | 2:B:180:THR:HG22 | 1.89                     | 0.55              |
| 2:L:512:ASP:HB3  | 2:L:514:TYR:CE1  | 2.41                     | 0.55              |
| 2:L:780:VAL:HG13 | 2:L:792:PHE:HE2  | 1.72                     | 0.55              |
| 2:L:77:THR:HB    | 2:L:78:TYR:CD1   | 2.42                     | 0.54              |
| 2:C:191:PRO:CG   | 2:C:281:TYR:CD2  | 2.90                     | 0.54              |
| 2:B:166:GLU:CB   | 2:B:184:PHE:CD2  | 2.90                     | 0.54              |
| 2:L:514:TYR:CD2  | 2:L:844:PRO:HG3  | 2.42                     | 0.54              |
| 2:L:890:LEU:C    | 2:L:891:TYR:CD1  | 2.85                     | 0.54              |
| 2:D:670:ALA:HB1  | 2:F:6:MET:HE1    | 1.89                     | 0.53              |
| 2:E:457:MET:HE2  | 2:F:457:MET:HE2  | 1.89                     | 0.53              |
| 2:G:457:MET:HE3  | 2:I:457:MET:HE1  | 1.91                     | 0.53              |
| 2:B:545:MET:HE1  | 2:C:398:HIS:ND1  | 2.23                     | 0.53              |
| 2:F:332:TYR:CE1  | 2:F:583:ARG:HG2  | 2.43                     | 0.53              |
| 2:G:872:PHE:CZ   | 2:G:891:TYR:CE2  | 2.97                     | 0.53              |
| 2:E:433:GLU:C    | 2:E:434:GLU:HG3  | 2.34                     | 0.53              |
| 2:E:176:GLU:HG2  | 2:E:180:THR:HG23 | 1.91                     | 0.53              |
| 2:D:457:MET:HE2  | 2:F:457:MET:HE2  | 1.91                     | 0.52              |
| 2:E:142:THR:HG23 | 2:E:145:GLN:O    | 2.09                     | 0.52              |
| 2:G:84:PHE:CD2   | 2:G:612:LEU:CB   | 2.92                     | 0.52              |
| 2:L:430:ASP:C    | 2:L:432:ALA:H    | 2.16                     | 0.52              |
| 2:I:332:TYR:CE1  | 2:I:583:ARG:HG2  | 2.44                     | 0.52              |
| 2:D:613:TYR:CZ   | 2:E:760:LYS:HE2  | 2.45                     | 0.52              |
| 2:I:711:LEU:HD22 | 2:I:907:MET:HE1  | 1.92                     | 0.52              |
| 2:C:166:GLU:CB   | 2:C:184:PHE:CD2  | 2.93                     | 0.52              |
| 2:E:200:TRP:C    | 2:E:202:GLU:H    | 2.17                     | 0.51              |
| 2:D:20:ALA:HA    | 2:D:23:TYR:CE2   | 2.46                     | 0.51              |
| 2:A:825:PHE:CE2  | 2:C:125:ALA:HB2  | 2.45                     | 0.51              |
| 2:G:457:MET:CE   | 2:I:457:MET:HE1  | 2.41                     | 0.51              |
| 2:K:944:ALA:C    | 2:K:946:ASN:H    | 2.19                     | 0.51              |
| 2:A:327:PHE:CZ   | 2:A:382:ASN:HB2  | 2.46                     | 0.51              |
| 1:6:9:LEU:HG     | 1:6:10:ALA:H     | 1.75                     | 0.51              |
| 2:I:200:TRP:CE3  | 2:I:412:ASN:HB3  | 2.46                     | 0.51              |
| 2:A:890:LEU:HD21 | 2:C:7:MET:HE3    | 1.93                     | 0.50              |
| 2:F:270:GLN:H    | 2:F:273:GLU:HG3  | 1.76                     | 0.50              |
| 2:K:512:ASP:HB3  | 2:K:514:TYR:CE1  | 2.46                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:77:THR:HB    | 2:L:78:TYR:HD1   | 1.75                     | 0.50              |
| 2:D:457:MET:HE2  | 2:E:457:MET:HE2  | 1.93                     | 0.50              |
| 2:F:332:TYR:CD2  | 2:F:338:ASN:HB3  | 2.46                     | 0.50              |
| 2:I:664:ILE:HD11 | 2:I:669:TRP:CH2  | 2.47                     | 0.50              |
| 2:A:437:TRP:CD1  | 2:B:275:LYS:HA   | 2.46                     | 0.50              |
| 2:A:275:LYS:HA   | 2:C:437:TRP:CD1  | 2.47                     | 0.49              |
| 2:G:367:LEU:HA   | 2:G:643:TYR:CE2  | 2.46                     | 0.49              |
| 2:F:430:ASP:HB3  | 2:F:432:ALA:HB3  | 1.93                     | 0.49              |
| 2:I:84:PHE:CD2   | 2:I:612:LEU:CB   | 2.95                     | 0.49              |
| 2:I:327:PHE:CZ   | 2:I:382:ASN:HB2  | 2.48                     | 0.49              |
| 2:L:83:ARG:CD    | 2:L:577:THR:HG23 | 2.41                     | 0.49              |
| 2:G:83:ARG:C     | 2:G:84:PHE:HD1   | 2.21                     | 0.49              |
| 6:S:88:SER:H     | 6:S:89:PRO:HD2   | 1.77                     | 0.49              |
| 2:L:940:THR:HG23 | 2:L:941:PRO:HD3  | 1.93                     | 0.49              |
| 2:F:664:ILE:HD11 | 2:F:669:TRP:CH2  | 2.48                     | 0.49              |
| 2:L:710:TYR:CE1  | 2:L:711:LEU:HG   | 2.48                     | 0.49              |
| 2:D:457:MET:HG3  | 2:F:457:MET:HE1  | 1.94                     | 0.48              |
| 2:F:327:PHE:CZ   | 2:F:382:ASN:HB2  | 2.47                     | 0.48              |
| 2:K:940:THR:HG23 | 2:K:941:PRO:HD3  | 1.94                     | 0.48              |
| 2:E:200:TRP:CH2  | 2:F:310:THR:HA   | 2.49                     | 0.48              |
| 2:K:113:PHE:CZ   | 2:K:115:PRO:HG3  | 2.48                     | 0.48              |
| 2:K:583:ARG:O    | 2:K:589:ILE:HD11 | 2.13                     | 0.48              |
| 2:K:940:THR:HG23 | 2:K:941:PRO:CD   | 2.43                     | 0.48              |
| 2:L:940:THR:HG23 | 2:L:941:PRO:CD   | 2.43                     | 0.48              |
| 2:D:327:PHE:CZ   | 2:D:382:ASN:HB2  | 2.48                     | 0.48              |
| 2:K:327:PHE:CZ   | 2:K:382:ASN:HB2  | 2.48                     | 0.48              |
| 2:E:200:TRP:HE1  | 2:E:412:ASN:CA   | 2.25                     | 0.48              |
| 2:A:890:LEU:CD2  | 2:C:7:MET:HE3    | 2.43                     | 0.48              |
| 2:C:327:PHE:CZ   | 2:C:382:ASN:HB2  | 2.48                     | 0.48              |
| 2:L:113:PHE:CZ   | 2:L:115:PRO:CG   | 2.97                     | 0.48              |
| 2:L:327:PHE:CZ   | 2:L:382:ASN:HB2  | 2.49                     | 0.48              |
| 2:F:734:LEU:CB   | 2:F:737:PRO:HD2  | 2.44                     | 0.48              |
| 2:K:891:TYR:CD1  | 2:K:892:ALA:N    | 2.81                     | 0.48              |
| 2:F:332:TYR:CD2  | 2:F:338:ASN:CB   | 2.97                     | 0.48              |
| 2:L:698:TYR:CD1  | 2:L:699:SER:N    | 2.82                     | 0.48              |
| 1:5:10:ALA:HB1   | 1:5:11:PRO:CD    | 2.44                     | 0.47              |
| 2:B:327:PHE:CZ   | 2:B:382:ASN:HB2  | 2.50                     | 0.47              |
| 2:C:266:THR:H    | 2:C:270:GLN:HB2  | 1.79                     | 0.47              |
| 2:E:327:PHE:CZ   | 2:E:382:ASN:HB2  | 2.49                     | 0.47              |
| 2:B:441:GLU:HG3  | 2:C:147:LYS:HE2  | 1.96                     | 0.47              |
| 2:I:83:ARG:C     | 2:I:84:PHE:HD1   | 2.22                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:332:TYR:CD2  | 2:I:338:ASN:CB   | 2.98                     | 0.47              |
| 2:J:113:PHE:CZ   | 2:J:115:PRO:CG   | 2.98                     | 0.47              |
| 2:J:940:THR:HG23 | 2:J:941:PRO:CD   | 2.45                     | 0.47              |
| 2:K:188:THR:HG21 | 2:K:250:TYR:CD2  | 2.50                     | 0.47              |
| 2:L:936:VAL:HG23 | 5:O:40:MET:HE3   | 1.96                     | 0.47              |
| 2:L:188:THR:HG21 | 2:L:250:TYR:CD2  | 2.50                     | 0.47              |
| 2:G:176:GLU:C    | 2:G:178:ASN:H    | 2.22                     | 0.47              |
| 1:7:22:TRP:CG    | 1:7:23:ASN:H     | 2.33                     | 0.47              |
| 2:L:78:TYR:CD2   | 2:L:692:PHE:CG   | 3.02                     | 0.47              |
| 2:L:781:PRO:HD2  | 2:L:792:PHE:CD2  | 2.50                     | 0.46              |
| 2:F:138:ASN:HA   | 2:F:148:SER:HA   | 1.97                     | 0.46              |
| 2:J:457:MET:HG3  | 2:L:457:MET:HE1  | 1.97                     | 0.46              |
| 5:O:10:MET:HE2   | 5:O:194:PRO:HB3  | 1.97                     | 0.46              |
| 2:L:919:VAL:HG12 | 2:L:941:PRO:HG2  | 1.96                     | 0.46              |
| 2:B:84:PHE:CD2   | 2:B:612:LEU:HB3  | 2.51                     | 0.46              |
| 2:K:919:VAL:HG12 | 2:K:941:PRO:HG2  | 1.97                     | 0.46              |
| 1:1:13:HIS:CG    | 1:1:14:GLY:N     | 2.82                     | 0.46              |
| 2:J:940:THR:HG23 | 2:J:941:PRO:HD3  | 1.98                     | 0.46              |
| 2:E:176:GLU:CG   | 2:E:180:THR:HG23 | 2.46                     | 0.46              |
| 2:G:872:PHE:HZ   | 2:G:891:TYR:CE2  | 2.34                     | 0.45              |
| 2:K:113:PHE:CZ   | 2:K:115:PRO:CG   | 2.99                     | 0.45              |
| 2:B:166:GLU:HB2  | 2:B:184:PHE:CD2  | 2.51                     | 0.45              |
| 2:F:265:PRO:HG3  | 2:F:270:GLN:C    | 2.41                     | 0.45              |
| 2:K:600:VAL:HG12 | 2:K:601:ASP:H    | 1.81                     | 0.45              |
| 2:K:887:GLN:HA   | 2:K:890:LEU:HD12 | 1.98                     | 0.45              |
| 2:B:84:PHE:CE2   | 2:B:612:LEU:CB   | 2.99                     | 0.45              |
| 2:E:889:MET:C    | 2:E:891:TYR:N    | 2.75                     | 0.45              |
| 2:I:737:PRO:HB2  | 2:I:739:GLU:H    | 1.80                     | 0.45              |
| 2:L:698:TYR:CE1  | 2:L:700:GLY:N    | 2.85                     | 0.45              |
| 2:B:701:SER:HB3  | 2:B:708:THR:CG2  | 2.47                     | 0.45              |
| 3:M:64:ALA:HA    | 3:M:67:ALA:HB3   | 1.98                     | 0.45              |
| 2:E:892:ALA:O    | 2:I:346:ALA:HB1  | 2.17                     | 0.45              |
| 2:K:189:PHE:CD1  | 2:K:189:PHE:N    | 2.83                     | 0.45              |
| 1:3:12:ARG:H     | 1:3:13:HIS:CD2   | 2.35                     | 0.45              |
| 1:8:8:SER:C      | 1:8:9:LEU:HD22   | 2.42                     | 0.45              |
| 2:L:698:TYR:CD1  | 2:L:698:TYR:C    | 2.95                     | 0.44              |
| 2:D:107:LEU:HD23 | 2:D:605:VAL:HG22 | 1.98                     | 0.44              |
| 2:F:734:LEU:HB2  | 2:F:737:PRO:CB   | 2.46                     | 0.44              |
| 2:I:736:THR:N    | 2:I:737:PRO:HD3  | 2.28                     | 0.44              |
| 2:B:84:PHE:CD2   | 2:B:612:LEU:CB   | 3.00                     | 0.44              |
| 2:E:176:GLU:C    | 2:E:178:ASN:N    | 2.75                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:323:PHE:CZ   | 2:F:555:PHE:CE2  | 3.06                     | 0.44              |
| 2:L:684:GLU:HG2  | 2:L:698:TYR:CE2  | 2.52                     | 0.44              |
| 2:E:320:TYR:HE2  | 2:E:541:ARG:HG2  | 1.82                     | 0.44              |
| 2:F:200:TRP:C    | 2:F:202:GLU:H    | 2.25                     | 0.44              |
| 2:L:681:LYS:HA   | 2:L:911:THR:HG22 | 2.00                     | 0.44              |
| 2:E:269:GLY:H    | 2:E:273:GLU:HB3  | 1.83                     | 0.44              |
| 2:A:895:ALA:HB2  | 2:L:346:ALA:HB2  | 2.00                     | 0.44              |
| 2:L:332:TYR:CD2  | 2:L:338:ASN:CB   | 3.01                     | 0.44              |
| 2:C:84:PHE:CD2   | 2:C:612:LEU:CB   | 3.01                     | 0.43              |
| 2:I:332:TYR:CD2  | 2:I:338:ASN:HB3  | 2.53                     | 0.43              |
| 1:5:1:MET:SD     | 2:G:869:ARG:HD3  | 2.58                     | 0.43              |
| 2:B:84:PHE:CE2   | 2:B:612:LEU:HB3  | 2.54                     | 0.43              |
| 2:E:887:GLN:HA   | 2:E:890:LEU:CD1  | 2.48                     | 0.43              |
| 2:E:202:GLU:O    | 2:E:203:THR:HB   | 2.18                     | 0.43              |
| 2:G:84:PHE:HD2   | 2:G:612:LEU:HB2  | 1.82                     | 0.43              |
| 2:G:327:PHE:CZ   | 2:G:382:ASN:HB2  | 2.54                     | 0.43              |
| 2:I:82:ALA:HB1   | 2:I:84:PHE:HE1   | 1.83                     | 0.43              |
| 2:E:52:PRO:HG2   | 2:E:56:VAL:HG21  | 1.99                     | 0.43              |
| 2:G:711:LEU:HD22 | 2:G:907:MET:HE1  | 2.01                     | 0.43              |
| 2:L:583:ARG:O    | 2:L:589:ILE:HD11 | 2.19                     | 0.43              |
| 2:L:890:LEU:HB2  | 2:L:891:TYR:CZ   | 2.53                     | 0.43              |
| 2:G:135:TRP:CZ2  | 2:G:151:GLN:HG3  | 2.54                     | 0.43              |
| 2:I:84:PHE:HD2   | 2:I:612:LEU:HB2  | 1.81                     | 0.43              |
| 2:K:681:LYS:HA   | 2:K:911:THR:HG22 | 2.00                     | 0.43              |
| 2:L:189:PHE:CD1  | 2:L:189:PHE:N    | 2.86                     | 0.43              |
| 2:C:166:GLU:CB   | 2:C:184:PHE:CE2  | 3.02                     | 0.43              |
| 2:E:320:TYR:CD1  | 2:E:320:TYR:N    | 2.87                     | 0.43              |
| 2:E:521:TRP:CE2  | 2:E:860:LYS:HE2  | 2.53                     | 0.43              |
| 2:I:894:SER:HB2  | 5:P:188:PHE:CE2  | 2.53                     | 0.43              |
| 2:C:84:PHE:CD2   | 2:C:612:LEU:HB3  | 2.53                     | 0.43              |
| 2:G:142:THR:CG2  | 2:G:143:GLY:N    | 2.82                     | 0.43              |
| 2:L:944:ALA:C    | 2:L:946:ASN:H    | 2.27                     | 0.43              |
| 2:A:457:MET:SD   | 2:B:457:MET:HE3  | 2.59                     | 0.43              |
| 2:B:566:ILE:HD11 | 2:B:580:TRP:CH2  | 2.53                     | 0.43              |
| 2:J:629:ALA:HB2  | 5:P:89:VAL:HG11  | 2.01                     | 0.43              |
| 2:K:889:MET:N    | 2:K:891:TYR:CE2  | 2.87                     | 0.43              |
| 2:F:737:PRO:HA   | 2:F:739:GLU:H    | 1.83                     | 0.42              |
| 2:I:176:GLU:C    | 2:I:178:ASN:H    | 2.26                     | 0.42              |
| 2:I:677:PHE:CD1  | 2:I:868:TRP:HB2  | 2.54                     | 0.42              |
| 2:I:728:TRP:CG   | 2:I:729:PRO:HA   | 2.54                     | 0.42              |
| 2:J:919:VAL:HG12 | 2:J:941:PRO:HG2  | 2.00                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:720:ILE:HG23 | 2:F:898:LEU:HD11 | 2.00                     | 0.42              |
| 2:G:82:ALA:HB1   | 2:G:84:PHE:HE1   | 1.85                     | 0.42              |
| 1:4:15:THR:HG22  | 1:4:16:ARG:N     | 2.32                     | 0.42              |
| 2:E:433:GLU:C    | 2:E:434:GLU:CG   | 2.91                     | 0.42              |
| 2:J:189:PHE:CD1  | 2:J:189:PHE:N    | 2.86                     | 0.42              |
| 2:B:457:MET:HE1  | 2:C:457:MET:SD   | 2.59                     | 0.42              |
| 2:A:125:ALA:HB2  | 2:B:825:PHE:CE2  | 2.55                     | 0.42              |
| 6:S:76:ARG:C     | 6:S:76:ARG:HD2   | 2.44                     | 0.42              |
| 2:D:720:ILE:HG23 | 2:D:898:LEU:HD11 | 2.02                     | 0.42              |
| 2:G:907:MET:HG2  | 2:G:911:THR:HG21 | 2.02                     | 0.42              |
| 2:K:889:MET:HA   | 2:K:891:TYR:CE2  | 2.55                     | 0.42              |
| 2:C:135:TRP:CZ2  | 2:C:151:GLN:HG3  | 2.55                     | 0.42              |
| 2:F:806:ILE:HD13 | 6:S:111:LEU:HB3  | 2.02                     | 0.42              |
| 2:H:457:MET:SD   | 2:I:457:MET:HE2  | 2.60                     | 0.42              |
| 2:B:756:CYS:SG   | 2:B:757:ASN:N    | 2.93                     | 0.42              |
| 2:F:107:LEU:CD2  | 2:F:605:VAL:HG22 | 2.48                     | 0.42              |
| 2:F:737:PRO:HA   | 2:F:739:GLU:N    | 2.34                     | 0.42              |
| 2:L:8:PRO:HD3    | 5:P:18:GLY:HA2   | 2.02                     | 0.42              |
| 2:L:943:SER:OG   | 5:O:28:SER:C     | 2.63                     | 0.42              |
| 2:G:200:TRP:CE3  | 2:G:412:ASN:HB3  | 2.55                     | 0.42              |
| 2:H:681:LYS:HA   | 2:H:911:THR:HG22 | 2.02                     | 0.42              |
| 2:L:891:TYR:CD1  | 2:L:891:TYR:N    | 2.78                     | 0.42              |
| 2:A:366:LEU:HB3  | 2:A:644:LEU:HD13 | 2.01                     | 0.42              |
| 1:1:13:HIS:CG    | 1:1:14:GLY:H     | 2.38                     | 0.41              |
| 2:F:736:THR:H    | 2:F:737:PRO:HD2  | 1.85                     | 0.41              |
| 2:K:887:GLN:HA   | 2:K:890:LEU:CD1  | 2.50                     | 0.41              |
| 2:B:166:GLU:CB   | 2:B:184:PHE:CE2  | 3.03                     | 0.41              |
| 2:I:190:GLN:HA   | 2:I:191:PRO:C    | 2.45                     | 0.41              |
| 2:K:532:PHE:CD2  | 2:K:708:THR:HB   | 2.54                     | 0.41              |
| 2:L:263:THR:H    | 2:L:264:PRO:CD   | 2.32                     | 0.41              |
| 2:C:84:PHE:CE2   | 2:C:612:LEU:CB   | 3.03                     | 0.41              |
| 2:H:437:TRP:CD1  | 2:I:275:LYS:HA   | 2.55                     | 0.41              |
| 2:J:135:TRP:CZ2  | 2:J:151:GLN:HG3  | 2.55                     | 0.41              |
| 2:B:566:ILE:HD11 | 2:B:580:TRP:CZ3  | 2.55                     | 0.41              |
| 2:I:82:ALA:HB1   | 2:I:84:PHE:CE1   | 2.55                     | 0.41              |
| 2:L:135:TRP:CZ2  | 2:L:151:GLN:HG3  | 2.54                     | 0.41              |
| 2:I:264:PRO:HB2  | 2:I:265:PRO:HD2  | 2.01                     | 0.41              |
| 2:I:875:ASN:HD21 | 2:I:879:MET:HE2  | 1.84                     | 0.41              |
| 2:L:600:VAL:HG12 | 2:L:601:ASP:H    | 1.85                     | 0.41              |
| 1:3:8:SER:C      | 1:3:9:LEU:HD12   | 2.45                     | 0.41              |
| 2:D:521:TRP:CE2  | 2:D:860:LYS:HE2  | 2.56                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:893:ASN:HA   | 2:I:346:ALA:CB   | 2.50                     | 0.41              |
| 2:G:165:ILE:HD12 | 2:G:165:ILE:H    | 1.86                     | 0.41              |
| 2:G:178:ASN:CG   | 2:G:179:ALA:H    | 2.28                     | 0.41              |
| 2:J:843:PHE:CD1  | 2:J:843:PHE:C    | 2.99                     | 0.41              |
| 2:K:674:GLY:HA2  | 2:K:872:PHE:HB2  | 2.03                     | 0.41              |
| 2:L:320:TYR:HE2  | 2:L:541:ARG:HG2  | 1.82                     | 0.41              |
| 2:A:135:TRP:CZ2  | 2:A:151:GLN:HG3  | 2.56                     | 0.41              |
| 2:E:142:THR:HG21 | 2:E:145:GLN:HE21 | 1.85                     | 0.41              |
| 2:I:165:ILE:HD12 | 2:I:165:ILE:H    | 1.85                     | 0.41              |
| 2:I:332:TYR:HD2  | 2:I:338:ASN:HB3  | 1.85                     | 0.41              |
| 2:K:113:PHE:CE1  | 2:K:115:PRO:HG3  | 2.55                     | 0.41              |
| 2:K:888:ASN:O    | 2:K:889:MET:HG2  | 2.21                     | 0.41              |
| 2:K:892:ALA:O    | 2:K:894:SER:N    | 2.54                     | 0.41              |
| 2:L:893:ASN:HA   | 5:O:10:MET:SD    | 2.61                     | 0.41              |
| 2:E:720:ILE:HG23 | 2:E:898:LEU:HD11 | 2.02                     | 0.41              |
| 2:H:678:THR:HG21 | 2:H:709:PHE:CE1  | 2.56                     | 0.41              |
| 2:I:200:TRP:CD2  | 2:I:412:ASN:HB3  | 2.55                     | 0.41              |
| 2:L:521:TRP:CZ2  | 2:L:860:LYS:HE2  | 2.56                     | 0.41              |
| 2:D:52:PRO:HG2   | 2:D:56:VAL:HG21  | 2.03                     | 0.40              |
| 2:I:178:ASN:CG   | 2:I:179:ALA:H    | 2.30                     | 0.40              |
| 2:L:197:GLU:HB2  | 2:L:202:GLU:CD   | 2.46                     | 0.40              |
| 2:G:872:PHE:CZ   | 2:G:885:LEU:HB3  | 2.55                     | 0.40              |
| 2:I:434:GLU:HG3  | 2:I:436:GLU:H    | 1.87                     | 0.40              |
| 2:E:20:ALA:HA    | 2:E:23:TYR:CE2   | 2.57                     | 0.40              |
| 2:J:327:PHE:CZ   | 2:J:382:ASN:HB2  | 2.57                     | 0.40              |
| 2:J:521:TRP:CZ2  | 2:J:860:LYS:HE2  | 2.56                     | 0.40              |
| 2:F:261:GLY:C    | 2:F:263:THR:H    | 2.30                     | 0.40              |
| 3:M:237:PRO:HA   | 3:M:268:TYR:CG   | 2.57                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 1   | 1     | 20/234 (8%)       | 16 (80%)    | 4 (20%)  | 0        | 100         | 100 |
| 1   | 2     | 14/234 (6%)       | 9 (64%)     | 4 (29%)  | 1 (7%)   | 1           | 6   |
| 1   | 3     | 19/234 (8%)       | 9 (47%)     | 7 (37%)  | 3 (16%)  | 0           | 1   |
| 1   | 4     | 9/234 (4%)        | 4 (44%)     | 4 (44%)  | 1 (11%)  | 0           | 2   |
| 1   | 5     | 23/234 (10%)      | 14 (61%)    | 5 (22%)  | 4 (17%)  | 0           | 0   |
| 1   | 6     | 18/234 (8%)       | 10 (56%)    | 5 (28%)  | 3 (17%)  | 0           | 1   |
| 1   | 7     | 25/234 (11%)      | 17 (68%)    | 5 (20%)  | 3 (12%)  | 0           | 1   |
| 1   | 8     | 13/234 (6%)       | 8 (62%)     | 5 (38%)  | 0        | 100         | 100 |
| 2   | A     | 939/941 (100%)    | 883 (94%)   | 53 (6%)  | 3 (0%)   | 36          | 65  |
| 2   | B     | 939/941 (100%)    | 881 (94%)   | 49 (5%)  | 9 (1%)   | 12          | 40  |
| 2   | C     | 939/941 (100%)    | 886 (94%)   | 45 (5%)  | 8 (1%)   | 14          | 43  |
| 2   | D     | 939/941 (100%)    | 877 (93%)   | 59 (6%)  | 3 (0%)   | 36          | 65  |
| 2   | E     | 939/941 (100%)    | 866 (92%)   | 59 (6%)  | 14 (2%)  | 8           | 32  |
| 2   | F     | 939/941 (100%)    | 875 (93%)   | 53 (6%)  | 11 (1%)  | 10          | 37  |
| 2   | G     | 939/941 (100%)    | 881 (94%)   | 49 (5%)  | 9 (1%)   | 12          | 40  |
| 2   | H     | 939/941 (100%)    | 888 (95%)   | 50 (5%)  | 1 (0%)   | 48          | 75  |
| 2   | I     | 939/941 (100%)    | 879 (94%)   | 50 (5%)  | 10 (1%)  | 11          | 39  |
| 2   | J     | 939/941 (100%)    | 880 (94%)   | 54 (6%)  | 5 (0%)   | 24          | 55  |
| 2   | K     | 939/941 (100%)    | 879 (94%)   | 50 (5%)  | 10 (1%)  | 11          | 39  |
| 2   | L     | 937/941 (100%)    | 881 (94%)   | 48 (5%)  | 8 (1%)   | 14          | 43  |
| 3   | M     | 468/519 (90%)     | 438 (94%)   | 30 (6%)  | 0        | 100         | 100 |
| 4   | N     | 279/559 (50%)     | 254 (91%)   | 23 (8%)  | 2 (1%)   | 18          | 49  |
| 5   | O     | 173/227 (76%)     | 163 (94%)   | 10 (6%)  | 0        | 100         | 100 |
| 5   | P     | 176/227 (78%)     | 162 (92%)   | 14 (8%)  | 0        | 100         | 100 |
| 6   | Q     | 37/134 (28%)      | 37 (100%)   | 0        | 0        | 100         | 100 |
| 6   | R     | 34/134 (25%)      | 33 (97%)    | 1 (3%)   | 0        | 100         | 100 |
| 6   | S     | 67/134 (50%)      | 53 (79%)    | 10 (15%) | 4 (6%)   | 1           | 9   |
| 6   | T     | 30/134 (22%)      | 30 (100%)   | 0        | 0        | 100         | 100 |
| All | All   | 12671/15232 (83%) | 11813 (93%) | 746 (6%) | 112 (1%) | 16          | 43  |

All (112) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 3     | 16  | ARG  |
| 1   | 5     | 6   | PHE  |
| 1   | 6     | 10  | ALA  |
| 2   | B     | 268 | SER  |
| 2   | B     | 269 | GLY  |
| 2   | B     | 270 | GLN  |
| 2   | B     | 271 | GLN  |
| 2   | C     | 430 | ASP  |
| 2   | C     | 432 | ALA  |
| 2   | C     | 944 | ALA  |
| 2   | E     | 177 | GLY  |
| 2   | E     | 271 | GLN  |
| 2   | E     | 273 | GLU  |
| 2   | E     | 434 | GLU  |
| 2   | E     | 889 | MET  |
| 2   | F     | 137 | ALA  |
| 2   | F     | 138 | ASN  |
| 2   | F     | 261 | GLY  |
| 2   | F     | 271 | GLN  |
| 2   | F     | 434 | GLU  |
| 2   | G     | 142 | THR  |
| 2   | G     | 143 | GLY  |
| 2   | G     | 888 | ASN  |
| 2   | G     | 889 | MET  |
| 2   | I     | 268 | SER  |
| 2   | I     | 736 | THR  |
| 2   | I     | 888 | ASN  |
| 2   | K     | 431 | GLY  |
| 2   | K     | 433 | GLU  |
| 2   | K     | 893 | ASN  |
| 2   | L     | 433 | GLU  |
| 1   | 2     | 29  | GLN  |
| 1   | 7     | 18  | PHE  |
| 2   | E     | 203 | THR  |
| 2   | E     | 888 | ASN  |
| 2   | E     | 892 | ALA  |
| 2   | F     | 273 | GLU  |
| 2   | F     | 433 | GLU  |
| 2   | G     | 176 | GLU  |
| 2   | G     | 177 | GLY  |
| 2   | I     | 176 | GLU  |
| 2   | I     | 889 | MET  |
| 2   | K     | 429 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | L     | 889 | MET  |
| 2   | L     | 894 | SER  |
| 6   | S     | 74  | ALA  |
| 6   | S     | 83  | PRO  |
| 6   | S     | 88  | SER  |
| 1   | 3     | 5   | ASN  |
| 1   | 5     | 15  | THR  |
| 1   | 6     | 9   | LEU  |
| 2   | D     | 271 | GLN  |
| 2   | E     | 891 | TYR  |
| 2   | I     | 177 | GLY  |
| 2   | I     | 892 | ALA  |
| 2   | J     | 893 | ASN  |
| 2   | J     | 894 | SER  |
| 2   | K     | 8   | PRO  |
| 2   | K     | 864 | ASP  |
| 2   | K     | 889 | MET  |
| 2   | L     | 864 | ASP  |
| 4   | N     | 148 | PRO  |
| 1   | 5     | 19  | MET  |
| 2   | A     | 9   | GLN  |
| 2   | A     | 843 | PHE  |
| 2   | B     | 9   | GLN  |
| 2   | B     | 843 | PHE  |
| 2   | C     | 189 | PHE  |
| 2   | C     | 843 | PHE  |
| 2   | D     | 263 | THR  |
| 2   | E     | 175 | GLU  |
| 2   | E     | 202 | GLU  |
| 2   | F     | 141 | GLN  |
| 2   | J     | 864 | ASP  |
| 1   | 3     | 4   | ILE  |
| 1   | 4     | 17  | PRO  |
| 1   | 6     | 14  | GLY  |
| 2   | A     | 697 | VAL  |
| 2   | B     | 430 | ASP  |
| 2   | C     | 697 | VAL  |
| 2   | E     | 263 | THR  |
| 2   | E     | 348 | GLN  |
| 2   | F     | 736 | THR  |
| 2   | G     | 137 | ALA  |
| 2   | G     | 864 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | I     | 265 | PRO  |
| 2   | I     | 864 | ASP  |
| 2   | J     | 263 | THR  |
| 2   | L     | 263 | THR  |
| 1   | 5     | 10  | ALA  |
| 2   | B     | 189 | PHE  |
| 2   | B     | 697 | VAL  |
| 2   | C     | 601 | ASP  |
| 2   | K     | 894 | SER  |
| 2   | L     | 893 | ASN  |
| 2   | L     | 945 | GLY  |
| 4   | N     | 152 | PRO  |
| 6   | S     | 91  | VAL  |
| 1   | 7     | 10  | ALA  |
| 1   | 7     | 17  | PRO  |
| 2   | K     | 945 | GLY  |
| 2   | C     | 940 | THR  |
| 2   | E     | 697 | VAL  |
| 2   | J     | 941 | PRO  |
| 2   | D     | 697 | VAL  |
| 2   | F     | 697 | VAL  |
| 2   | L     | 843 | PHE  |
| 2   | G     | 265 | PRO  |
| 2   | H     | 265 | PRO  |
| 2   | I     | 737 | PRO  |
| 2   | K     | 263 | THR  |
| 2   | F     | 263 | THR  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed    | Rotameric | Outliers | Percentiles |    |
|-----|-------|-------------|-----------|----------|-------------|----|
| 1   | 1     | 18/195 (9%) | 14 (78%)  | 4 (22%)  | 1           | 5  |
| 1   | 2     | 11/195 (6%) | 10 (91%)  | 1 (9%)   | 9           | 31 |
| 1   | 3     | 17/195 (9%) | 15 (88%)  | 2 (12%)  | 5           | 20 |

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| Mol | Chain | Analysed          | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|-------------|-----|
| 1   | 4     | 9/195 (5%)        | 7 (78%)     | 2 (22%)  | 1           | 5   |
| 1   | 5     | 21/195 (11%)      | 17 (81%)    | 4 (19%)  | 1           | 7   |
| 1   | 6     | 16/195 (8%)       | 15 (94%)    | 1 (6%)   | 16          | 44  |
| 1   | 7     | 22/195 (11%)      | 18 (82%)    | 4 (18%)  | 2           | 8   |
| 1   | 8     | 14/195 (7%)       | 14 (100%)   | 0        | 100         | 100 |
| 2   | A     | 813/813 (100%)    | 805 (99%)   | 8 (1%)   | 68          | 76  |
| 2   | B     | 813/813 (100%)    | 804 (99%)   | 9 (1%)   | 65          | 76  |
| 2   | C     | 813/813 (100%)    | 801 (98%)   | 12 (2%)  | 57          | 72  |
| 2   | D     | 813/813 (100%)    | 805 (99%)   | 8 (1%)   | 68          | 76  |
| 2   | E     | 813/813 (100%)    | 802 (99%)   | 11 (1%)  | 59          | 73  |
| 2   | F     | 813/813 (100%)    | 804 (99%)   | 9 (1%)   | 65          | 76  |
| 2   | G     | 813/813 (100%)    | 807 (99%)   | 6 (1%)   | 76          | 80  |
| 2   | H     | 813/813 (100%)    | 807 (99%)   | 6 (1%)   | 76          | 80  |
| 2   | I     | 813/813 (100%)    | 807 (99%)   | 6 (1%)   | 76          | 80  |
| 2   | J     | 813/813 (100%)    | 809 (100%)  | 4 (0%)   | 81          | 83  |
| 2   | K     | 813/813 (100%)    | 809 (100%)  | 4 (0%)   | 81          | 83  |
| 2   | L     | 811/813 (100%)    | 798 (98%)   | 13 (2%)  | 55          | 72  |
| 3   | M     | 426/461 (92%)     | 420 (99%)   | 6 (1%)   | 59          | 73  |
| 4   | N     | 236/473 (50%)     | 233 (99%)   | 3 (1%)   | 61          | 74  |
| 5   | O     | 152/190 (80%)     | 150 (99%)   | 2 (1%)   | 61          | 74  |
| 5   | P     | 152/190 (80%)     | 147 (97%)   | 5 (3%)   | 33          | 59  |
| 6   | Q     | 33/102 (32%)      | 33 (100%)   | 0        | 100         | 100 |
| 6   | R     | 30/102 (29%)      | 29 (97%)    | 1 (3%)   | 33          | 59  |
| 6   | S     | 54/102 (53%)      | 51 (94%)    | 3 (6%)   | 19          | 47  |
| 6   | T     | 27/102 (26%)      | 25 (93%)    | 2 (7%)   | 13          | 38  |
| All | All   | 10992/13038 (84%) | 10856 (99%) | 136 (1%) | 61          | 75  |

All (136) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 9   | LEU  |
| 1   | 1     | 16  | ARG  |
| 1   | 1     | 19  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 23  | ASN  |
| 1   | 2     | 29  | GLN  |
| 1   | 3     | 6   | PHE  |
| 1   | 3     | 19  | MET  |
| 1   | 4     | 16  | ARG  |
| 1   | 4     | 22  | TRP  |
| 1   | 5     | 1   | MET  |
| 1   | 5     | 4   | ILE  |
| 1   | 5     | 12  | ARG  |
| 1   | 5     | 25  | ILE  |
| 1   | 6     | 18  | PHE  |
| 1   | 7     | 5   | ASN  |
| 1   | 7     | 16  | ARG  |
| 1   | 7     | 19  | MET  |
| 1   | 7     | 29  | GLN  |
| 2   | A     | 334 | ASN  |
| 2   | A     | 367 | LEU  |
| 2   | A     | 417 | ASN  |
| 2   | A     | 643 | TYR  |
| 2   | A     | 708 | THR  |
| 2   | A     | 738 | ASN  |
| 2   | A     | 848 | ILE  |
| 2   | A     | 919 | VAL  |
| 2   | B     | 84  | PHE  |
| 2   | B     | 334 | ASN  |
| 2   | B     | 367 | LEU  |
| 2   | B     | 417 | ASN  |
| 2   | B     | 580 | TRP  |
| 2   | B     | 581 | ASN  |
| 2   | B     | 643 | TYR  |
| 2   | B     | 867 | MET  |
| 2   | B     | 919 | VAL  |
| 2   | C     | 38  | TYR  |
| 2   | C     | 84  | PHE  |
| 2   | C     | 92  | ARG  |
| 2   | C     | 367 | LEU  |
| 2   | C     | 408 | CYS  |
| 2   | C     | 417 | ASN  |
| 2   | C     | 580 | TRP  |
| 2   | C     | 643 | TYR  |
| 2   | C     | 698 | TYR  |
| 2   | C     | 708 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 919 | VAL  |
| 2   | C     | 943 | SER  |
| 2   | D     | 13  | MET  |
| 2   | D     | 139 | GLU  |
| 2   | D     | 145 | GLN  |
| 2   | D     | 215 | ASP  |
| 2   | D     | 240 | LEU  |
| 2   | D     | 353 | VAL  |
| 2   | D     | 536 | ARG  |
| 2   | D     | 641 | ASN  |
| 2   | E     | 139 | GLU  |
| 2   | E     | 145 | GLN  |
| 2   | E     | 200 | TRP  |
| 2   | E     | 202 | GLU  |
| 2   | E     | 215 | ASP  |
| 2   | E     | 240 | LEU  |
| 2   | E     | 348 | GLN  |
| 2   | E     | 536 | ARG  |
| 2   | E     | 641 | ASN  |
| 2   | E     | 664 | ILE  |
| 2   | E     | 946 | ASN  |
| 2   | F     | 13  | MET  |
| 2   | F     | 139 | GLU  |
| 2   | F     | 145 | GLN  |
| 2   | F     | 202 | GLU  |
| 2   | F     | 215 | ASP  |
| 2   | F     | 240 | LEU  |
| 2   | F     | 536 | ARG  |
| 2   | F     | 555 | PHE  |
| 2   | F     | 737 | PRO  |
| 2   | G     | 272 | GLU  |
| 2   | G     | 273 | GLU  |
| 2   | G     | 286 | ASN  |
| 2   | G     | 398 | HIS  |
| 2   | G     | 664 | ILE  |
| 2   | G     | 802 | VAL  |
| 2   | H     | 181 | GLU  |
| 2   | H     | 200 | TRP  |
| 2   | H     | 273 | GLU  |
| 2   | H     | 286 | ASN  |
| 2   | H     | 398 | HIS  |
| 2   | H     | 802 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | I     | 181 | GLU  |
| 2   | I     | 200 | TRP  |
| 2   | I     | 286 | ASN  |
| 2   | I     | 398 | HIS  |
| 2   | I     | 677 | PHE  |
| 2   | I     | 802 | VAL  |
| 2   | J     | 7   | MET  |
| 2   | J     | 201 | GLN  |
| 2   | J     | 275 | LYS  |
| 2   | J     | 433 | GLU  |
| 2   | K     | 7   | MET  |
| 2   | K     | 181 | GLU  |
| 2   | K     | 433 | GLU  |
| 2   | K     | 514 | TYR  |
| 2   | L     | 78  | TYR  |
| 2   | L     | 201 | GLN  |
| 2   | L     | 202 | GLU  |
| 2   | L     | 275 | LYS  |
| 2   | L     | 408 | CYS  |
| 2   | L     | 430 | ASP  |
| 2   | L     | 433 | GLU  |
| 2   | L     | 514 | TYR  |
| 2   | L     | 570 | LEU  |
| 2   | L     | 580 | TRP  |
| 2   | L     | 698 | TYR  |
| 2   | L     | 710 | TYR  |
| 2   | L     | 890 | LEU  |
| 3   | M     | 52  | ASP  |
| 3   | M     | 341 | ASN  |
| 3   | M     | 383 | GLU  |
| 3   | M     | 385 | VAL  |
| 3   | M     | 401 | SER  |
| 3   | M     | 441 | THR  |
| 4   | N     | 91  | LEU  |
| 4   | N     | 178 | TYR  |
| 4   | N     | 195 | THR  |
| 5   | O     | 106 | VAL  |
| 5   | O     | 211 | GLU  |
| 5   | P     | 4   | GLU  |
| 5   | P     | 34  | LEU  |
| 5   | P     | 69  | LEU  |
| 5   | P     | 106 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | P     | 168 | TYR  |
| 6   | R     | 114 | GLN  |
| 6   | S     | 60  | ASP  |
| 6   | S     | 76  | ARG  |
| 6   | S     | 91  | VAL  |
| 6   | T     | 107 | GLU  |
| 6   | T     | 121 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (175) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 3     | 13  | HIS  |
| 1   | 8     | 5   | ASN  |
| 2   | A     | 14  | HIS  |
| 2   | A     | 18  | GLN  |
| 2   | A     | 54  | HIS  |
| 2   | A     | 131 | ASN  |
| 2   | A     | 235 | GLN  |
| 2   | A     | 284 | ASN  |
| 2   | A     | 286 | ASN  |
| 2   | A     | 311 | GLN  |
| 2   | A     | 338 | ASN  |
| 2   | A     | 345 | GLN  |
| 2   | A     | 365 | GLN  |
| 2   | A     | 417 | ASN  |
| 2   | A     | 448 | GLN  |
| 2   | A     | 464 | ASN  |
| 2   | A     | 581 | ASN  |
| 2   | A     | 648 | ASN  |
| 2   | A     | 659 | ASN  |
| 2   | A     | 757 | ASN  |
| 2   | A     | 794 | ASN  |
| 2   | A     | 893 | ASN  |
| 2   | A     | 896 | HIS  |
| 2   | A     | 926 | HIS  |
| 2   | B     | 9   | GLN  |
| 2   | B     | 14  | HIS  |
| 2   | B     | 131 | ASN  |
| 2   | B     | 235 | GLN  |
| 2   | B     | 286 | ASN  |
| 2   | B     | 326 | ASN  |
| 2   | B     | 338 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 365 | GLN  |
| 2   | B     | 406 | ASN  |
| 2   | B     | 464 | ASN  |
| 2   | B     | 581 | ASN  |
| 2   | B     | 648 | ASN  |
| 2   | B     | 757 | ASN  |
| 2   | B     | 770 | HIS  |
| 2   | B     | 794 | ASN  |
| 2   | C     | 18  | GLN  |
| 2   | C     | 134 | GLN  |
| 2   | C     | 235 | GLN  |
| 2   | C     | 270 | GLN  |
| 2   | C     | 284 | ASN  |
| 2   | C     | 286 | ASN  |
| 2   | C     | 311 | GLN  |
| 2   | C     | 326 | ASN  |
| 2   | C     | 338 | ASN  |
| 2   | C     | 365 | GLN  |
| 2   | C     | 406 | ASN  |
| 2   | C     | 417 | ASN  |
| 2   | C     | 448 | GLN  |
| 2   | C     | 581 | ASN  |
| 2   | C     | 587 | ASN  |
| 2   | C     | 757 | ASN  |
| 2   | C     | 794 | ASN  |
| 2   | C     | 893 | ASN  |
| 2   | D     | 14  | HIS  |
| 2   | D     | 345 | GLN  |
| 2   | D     | 447 | ASN  |
| 2   | D     | 528 | ASN  |
| 2   | E     | 134 | GLN  |
| 2   | E     | 145 | GLN  |
| 2   | E     | 284 | ASN  |
| 2   | E     | 326 | ASN  |
| 2   | E     | 365 | GLN  |
| 2   | E     | 417 | ASN  |
| 2   | E     | 558 | GLN  |
| 2   | E     | 581 | ASN  |
| 2   | E     | 641 | ASN  |
| 2   | E     | 807 | ASN  |
| 2   | E     | 819 | GLN  |
| 2   | E     | 946 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 134 | GLN  |
| 2   | F     | 178 | ASN  |
| 2   | F     | 326 | ASN  |
| 2   | F     | 345 | GLN  |
| 2   | F     | 348 | GLN  |
| 2   | F     | 417 | ASN  |
| 2   | F     | 447 | ASN  |
| 2   | F     | 528 | ASN  |
| 2   | F     | 558 | GLN  |
| 2   | F     | 581 | ASN  |
| 2   | F     | 819 | GLN  |
| 2   | F     | 946 | ASN  |
| 2   | G     | 131 | ASN  |
| 2   | G     | 134 | GLN  |
| 2   | G     | 190 | GLN  |
| 2   | G     | 241 | ASN  |
| 2   | G     | 271 | GLN  |
| 2   | G     | 286 | ASN  |
| 2   | G     | 338 | ASN  |
| 2   | G     | 398 | HIS  |
| 2   | G     | 406 | ASN  |
| 2   | G     | 464 | ASN  |
| 2   | G     | 581 | ASN  |
| 2   | G     | 611 | ASN  |
| 2   | G     | 794 | ASN  |
| 2   | G     | 835 | GLN  |
| 2   | H     | 14  | HIS  |
| 2   | H     | 131 | ASN  |
| 2   | H     | 134 | GLN  |
| 2   | H     | 190 | GLN  |
| 2   | H     | 201 | GLN  |
| 2   | H     | 338 | ASN  |
| 2   | H     | 382 | ASN  |
| 2   | H     | 406 | ASN  |
| 2   | H     | 464 | ASN  |
| 2   | H     | 496 | ASN  |
| 2   | H     | 794 | ASN  |
| 2   | I     | 131 | ASN  |
| 2   | I     | 134 | GLN  |
| 2   | I     | 235 | GLN  |
| 2   | I     | 241 | ASN  |
| 2   | I     | 406 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | I     | 464 | ASN  |
| 2   | I     | 581 | ASN  |
| 2   | I     | 766 | GLN  |
| 2   | I     | 835 | GLN  |
| 2   | I     | 893 | ASN  |
| 2   | J     | 14  | HIS  |
| 2   | J     | 18  | GLN  |
| 2   | J     | 62  | GLN  |
| 2   | J     | 134 | GLN  |
| 2   | J     | 178 | ASN  |
| 2   | J     | 201 | GLN  |
| 2   | J     | 326 | ASN  |
| 2   | J     | 338 | ASN  |
| 2   | J     | 365 | GLN  |
| 2   | J     | 488 | ASN  |
| 2   | J     | 558 | GLN  |
| 2   | J     | 633 | ASN  |
| 2   | J     | 926 | HIS  |
| 2   | K     | 134 | GLN  |
| 2   | K     | 286 | ASN  |
| 2   | K     | 338 | ASN  |
| 2   | K     | 348 | GLN  |
| 2   | K     | 365 | GLN  |
| 2   | K     | 488 | ASN  |
| 2   | K     | 558 | GLN  |
| 2   | K     | 611 | ASN  |
| 2   | K     | 926 | HIS  |
| 2   | L     | 131 | ASN  |
| 2   | L     | 134 | GLN  |
| 2   | L     | 178 | ASN  |
| 2   | L     | 201 | GLN  |
| 2   | L     | 286 | ASN  |
| 2   | L     | 326 | ASN  |
| 2   | L     | 338 | ASN  |
| 2   | L     | 348 | GLN  |
| 2   | L     | 365 | GLN  |
| 2   | L     | 464 | ASN  |
| 2   | L     | 488 | ASN  |
| 2   | L     | 659 | ASN  |
| 2   | L     | 926 | HIS  |
| 3   | M     | 117 | ASN  |
| 3   | M     | 120 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | M     | 179 | ASN  |
| 3   | M     | 191 | GLN  |
| 3   | M     | 347 | HIS  |
| 4   | N     | 46  | GLN  |
| 4   | N     | 68  | HIS  |
| 5   | O     | 14  | GLN  |
| 5   | O     | 53  | GLN  |
| 5   | O     | 166 | GLN  |
| 5   | O     | 199 | ASN  |
| 5   | P     | 103 | ASN  |
| 5   | P     | 172 | GLN  |
| 6   | Q     | 114 | GLN  |
| 6   | R     | 121 | GLN  |
| 6   | R     | 128 | GLN  |
| 6   | S     | 128 | GLN  |
| 6   | S     | 129 | GLN  |
| 6   | T     | 114 | GLN  |
| 6   | T     | 133 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

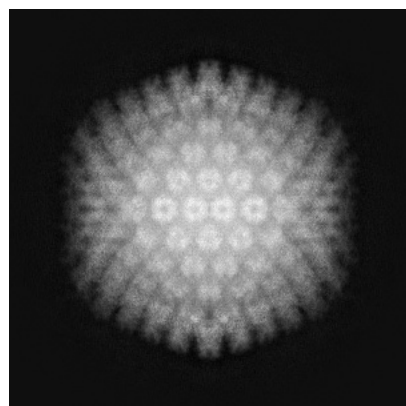
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53736. These allow visual inspection of the internal detail of the map and identification of artifacts.

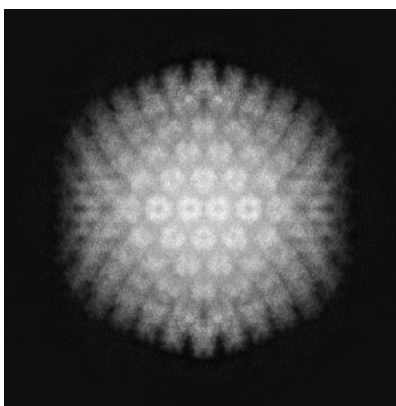
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

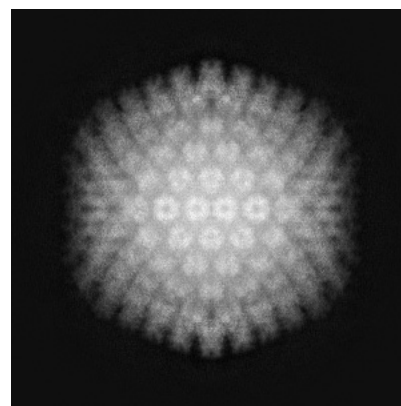
#### 6.1.1 Primary map



X

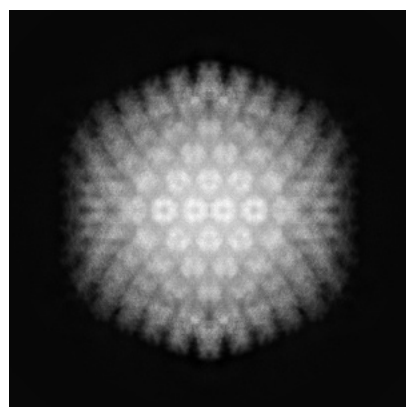


Y

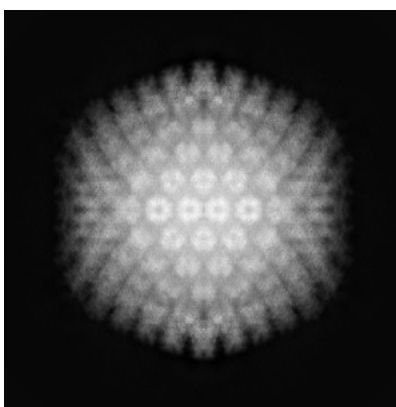


Z

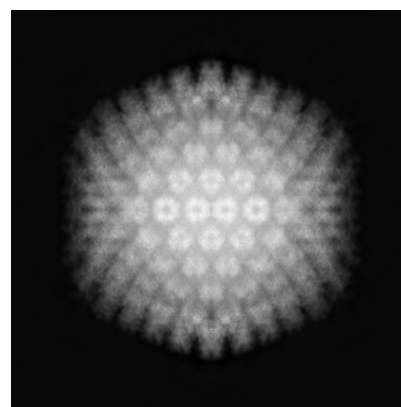
#### 6.1.2 Raw map



X



Y

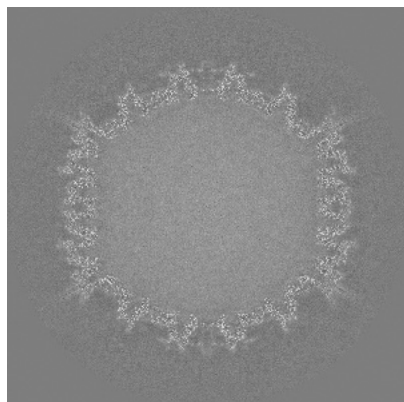


Z

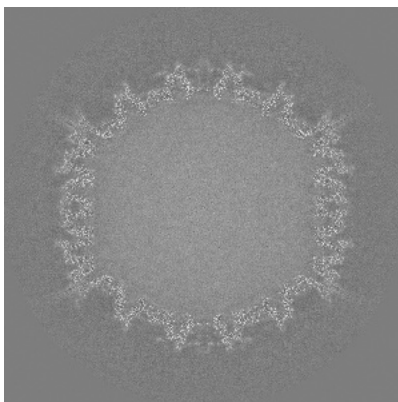
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

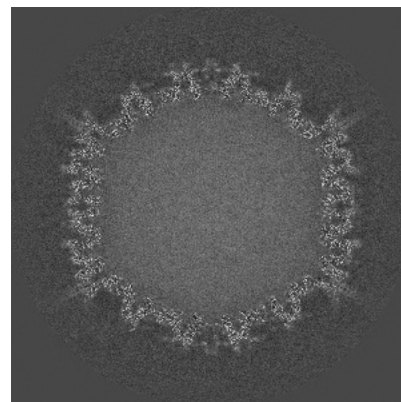
### 6.2.1 Primary map



X Index: 360

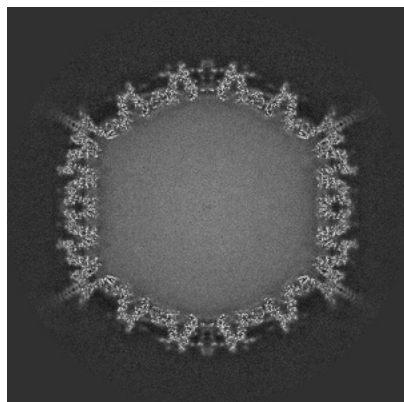


Y Index: 360

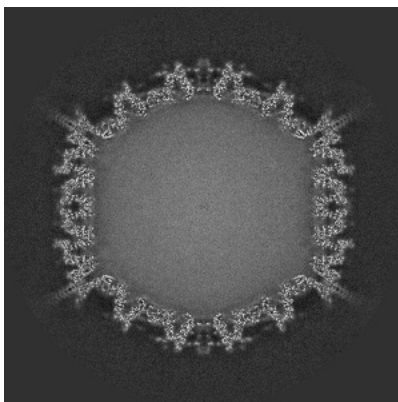


Z Index: 360

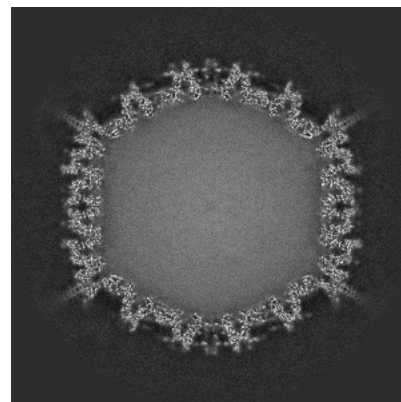
### 6.2.2 Raw map



X Index: 360



Y Index: 360

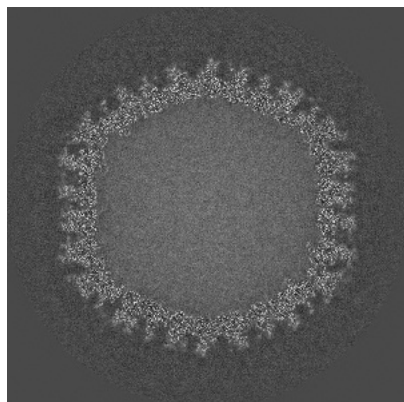


Z Index: 360

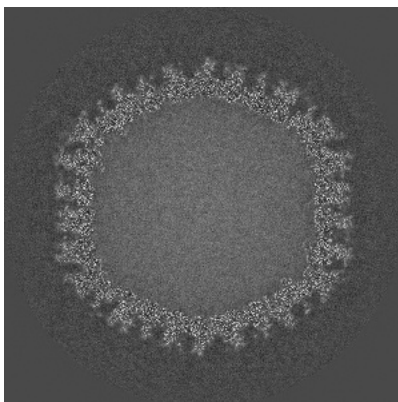
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

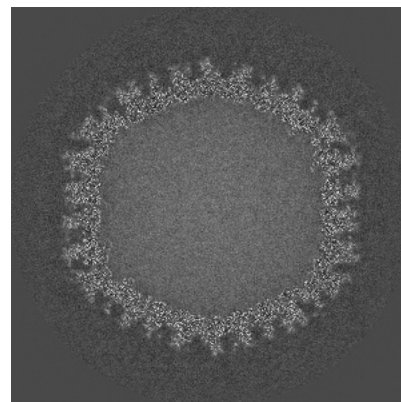
### 6.3.1 Primary map



X Index: 348

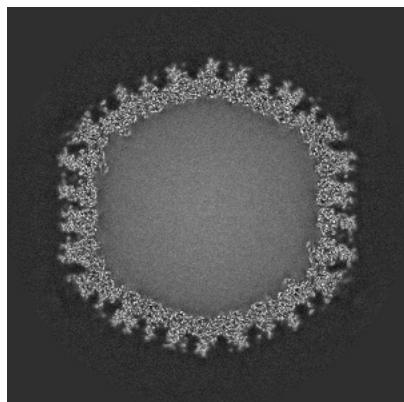


Y Index: 348

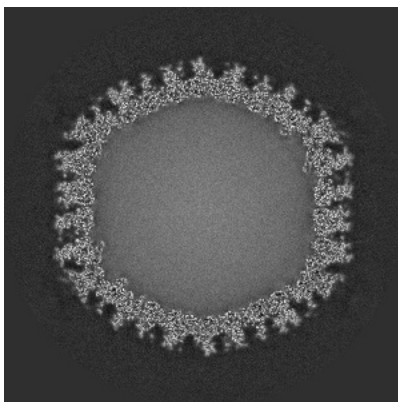


Z Index: 371

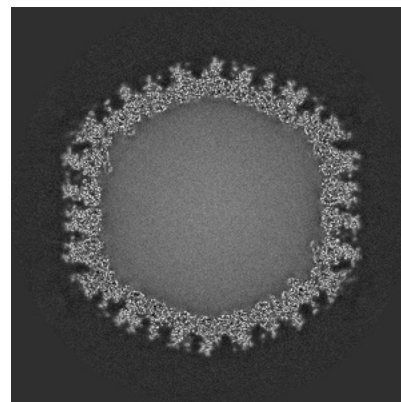
### 6.3.2 Raw map



X Index: 348



Y Index: 372



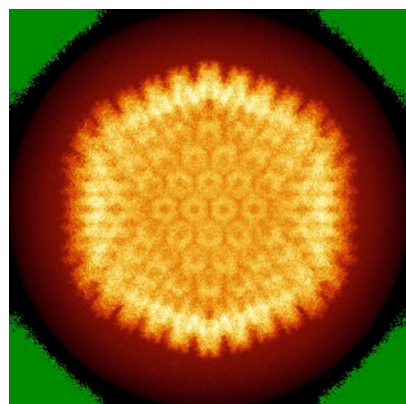
Z Index: 347

The images above show the largest variance slices of the map in three orthogonal directions.

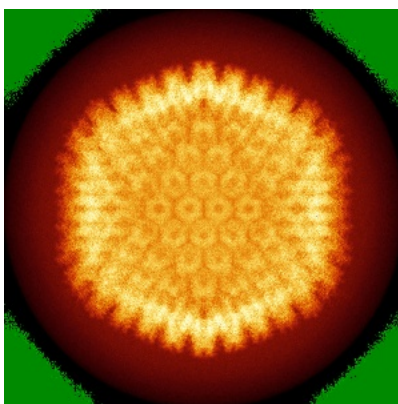


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

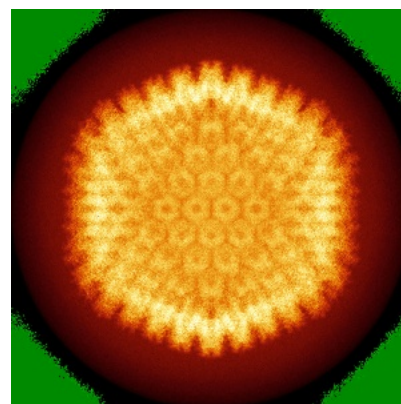
### 6.4.1 Primary map



X

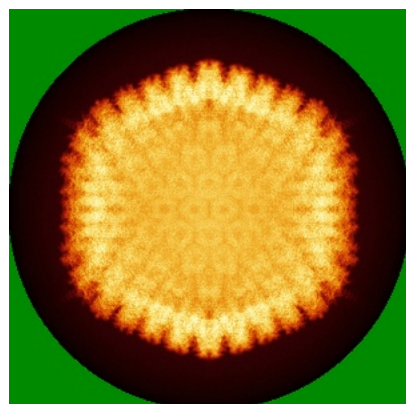


Y

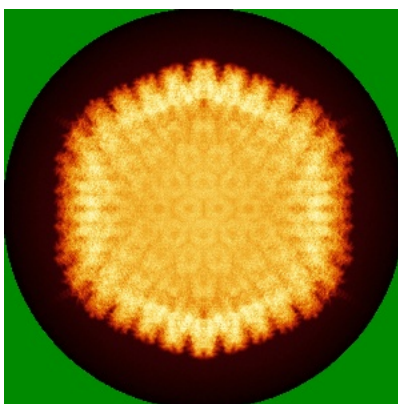


Z

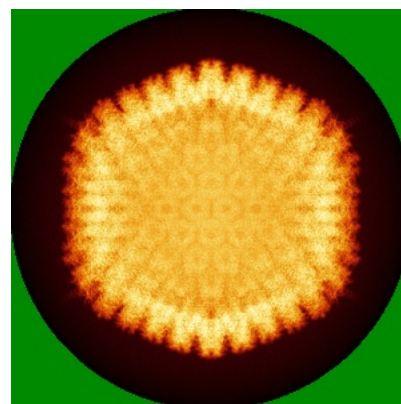
### 6.4.2 Raw map



X



Y

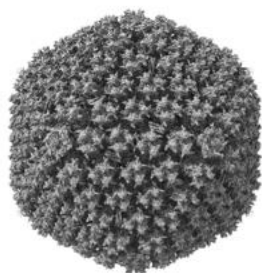


Z

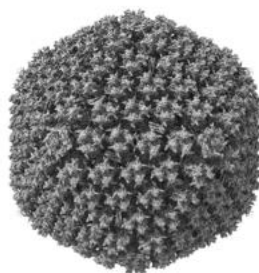
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

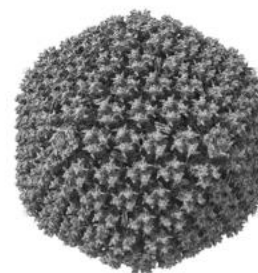
### 6.5.1 Primary map



X



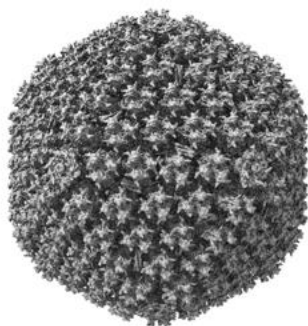
Y



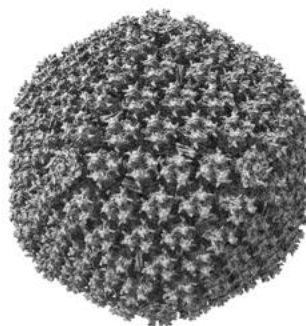
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0216. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

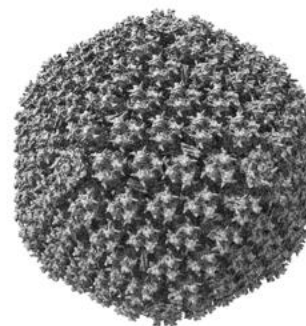
### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

## 6.6 Mask visualisation [i](#)

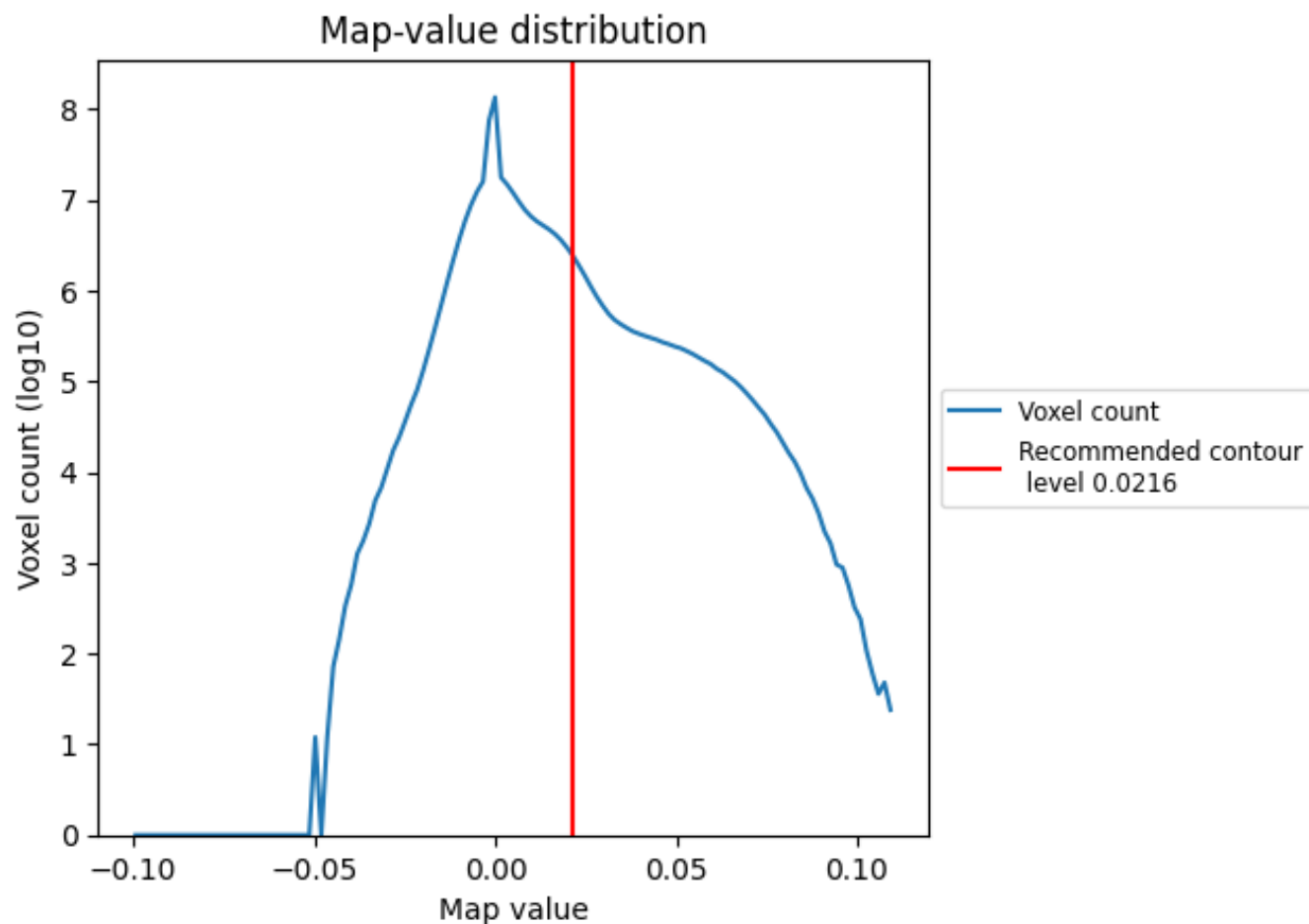
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

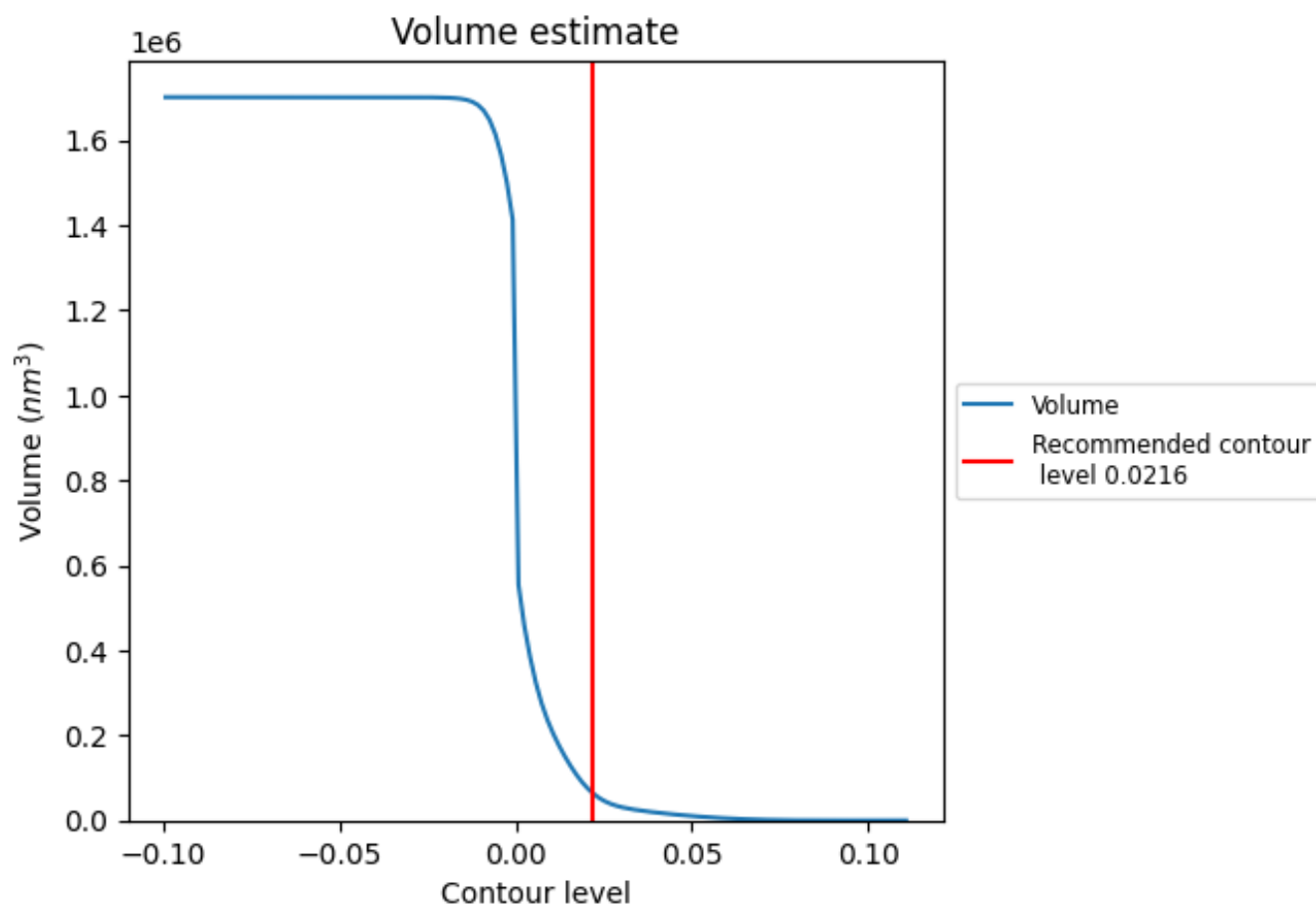
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

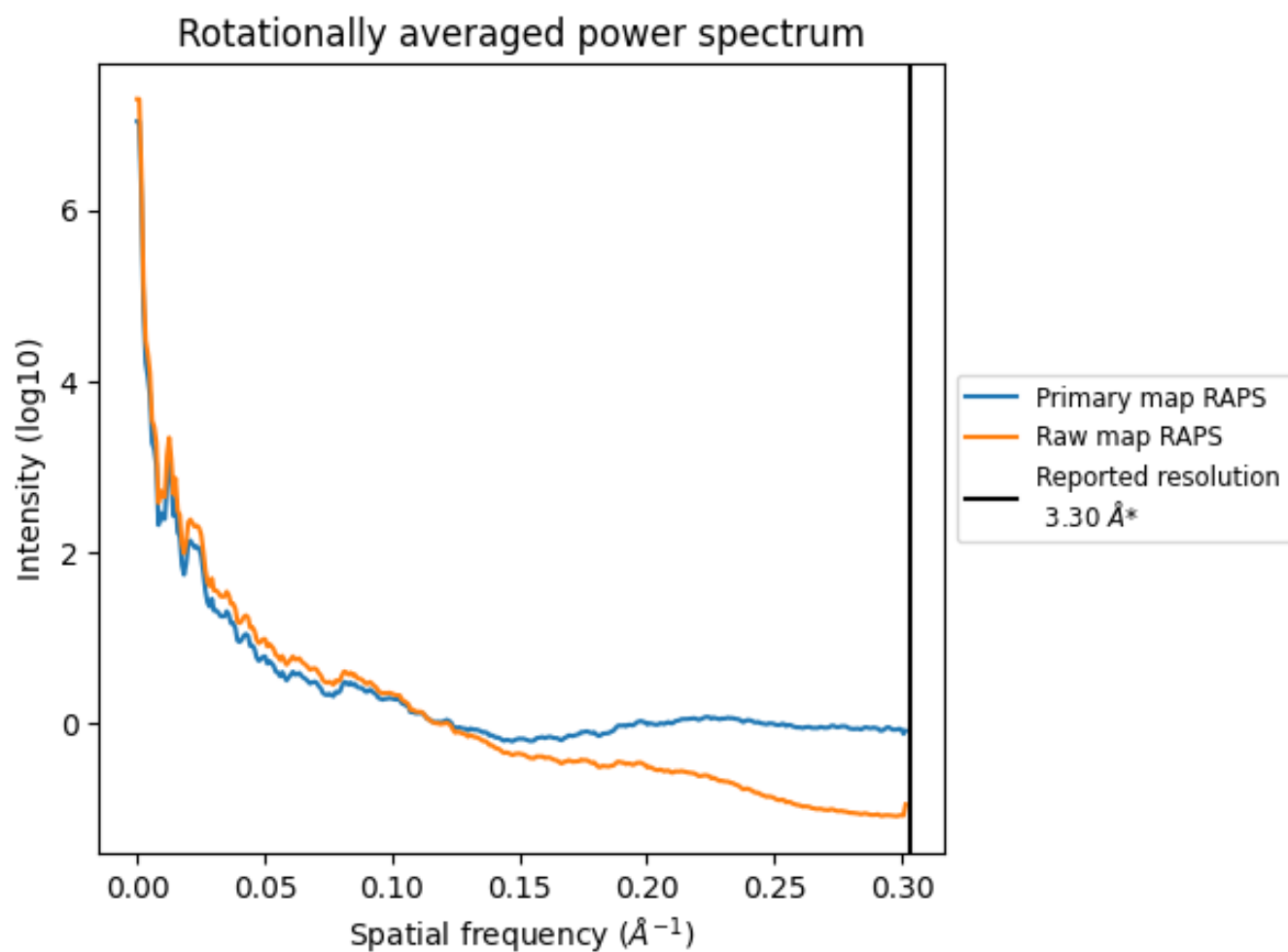
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 66526 nm<sup>3</sup>; this corresponds to an approximate mass of 60095 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

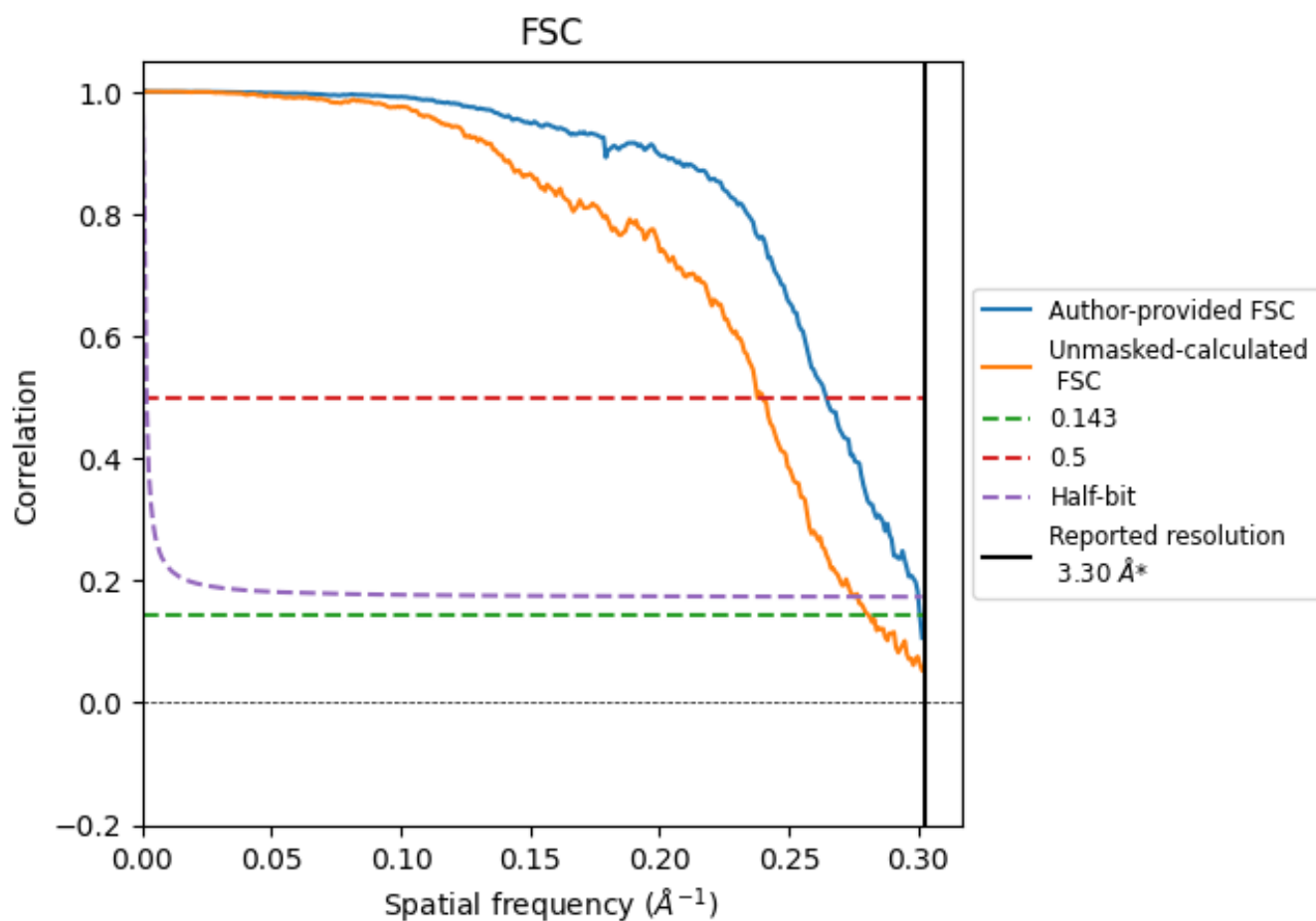


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.30                               | -    | -        |
| Author-provided FSC curve | 3.33                               | 3.78 | 3.33     |
| Unmasked-calculated*      | 3.56                               | 4.20 | 3.63     |

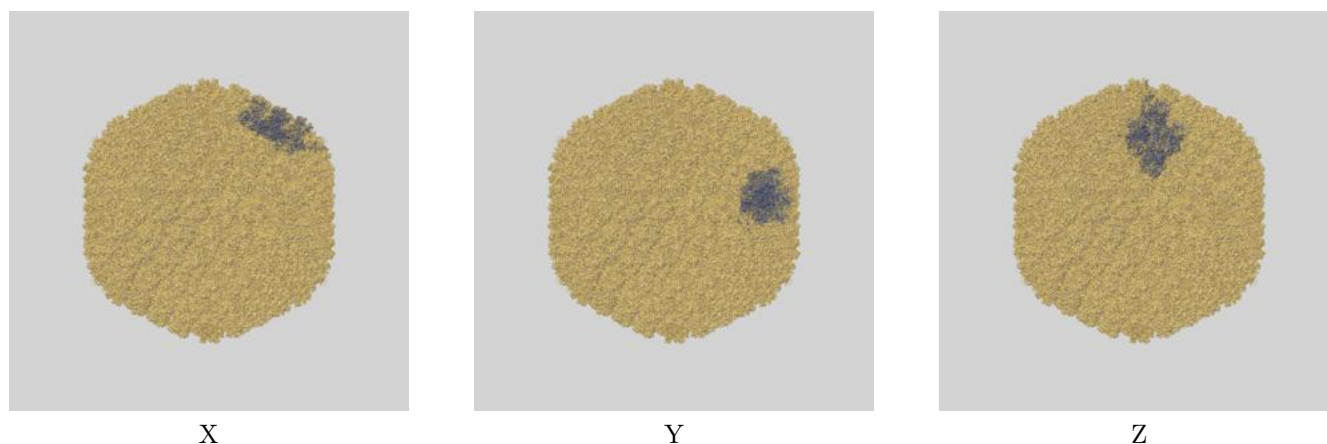
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

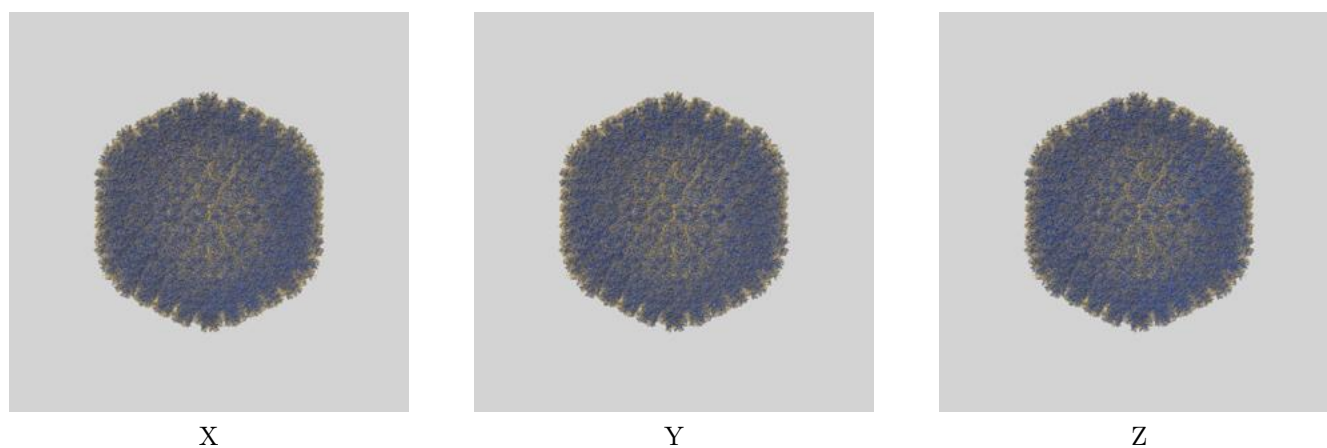
This section contains information regarding the fit between EMDB map EMD-53736 and PDB model 9R78. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlays

#### 9.1.1 Map-model overlay [i](#)

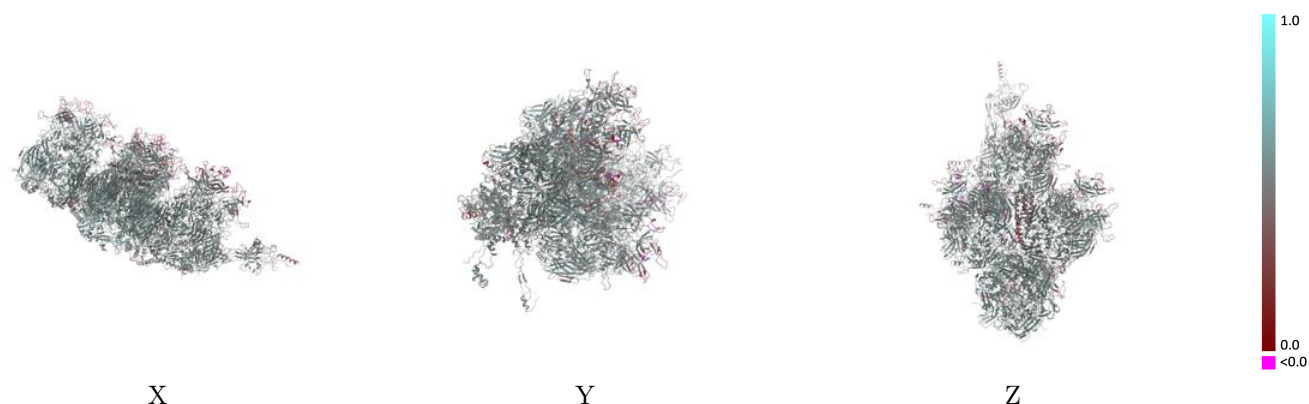


#### 9.1.2 Map-model assembly overlay [i](#)



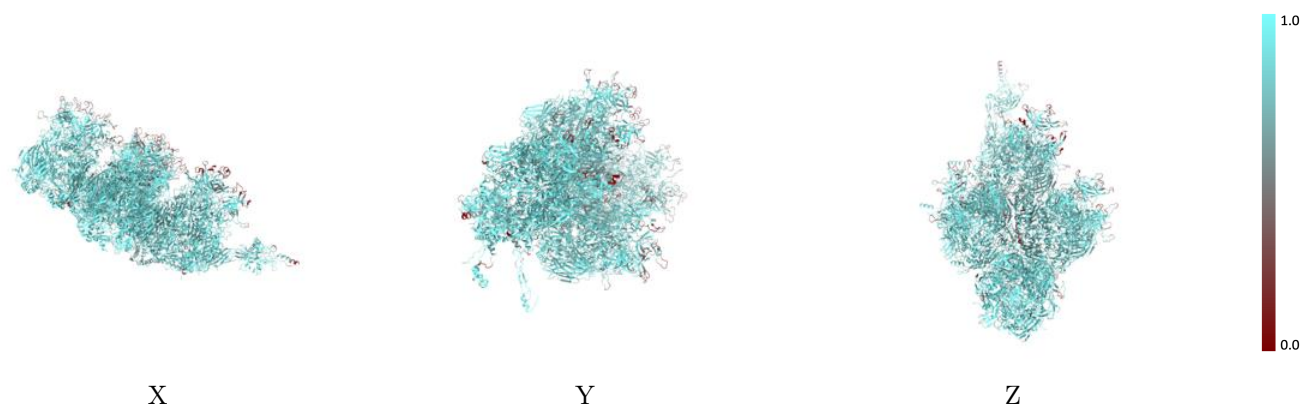
The images above show the 3D surface view of the map at the recommended contour level 0.0216 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



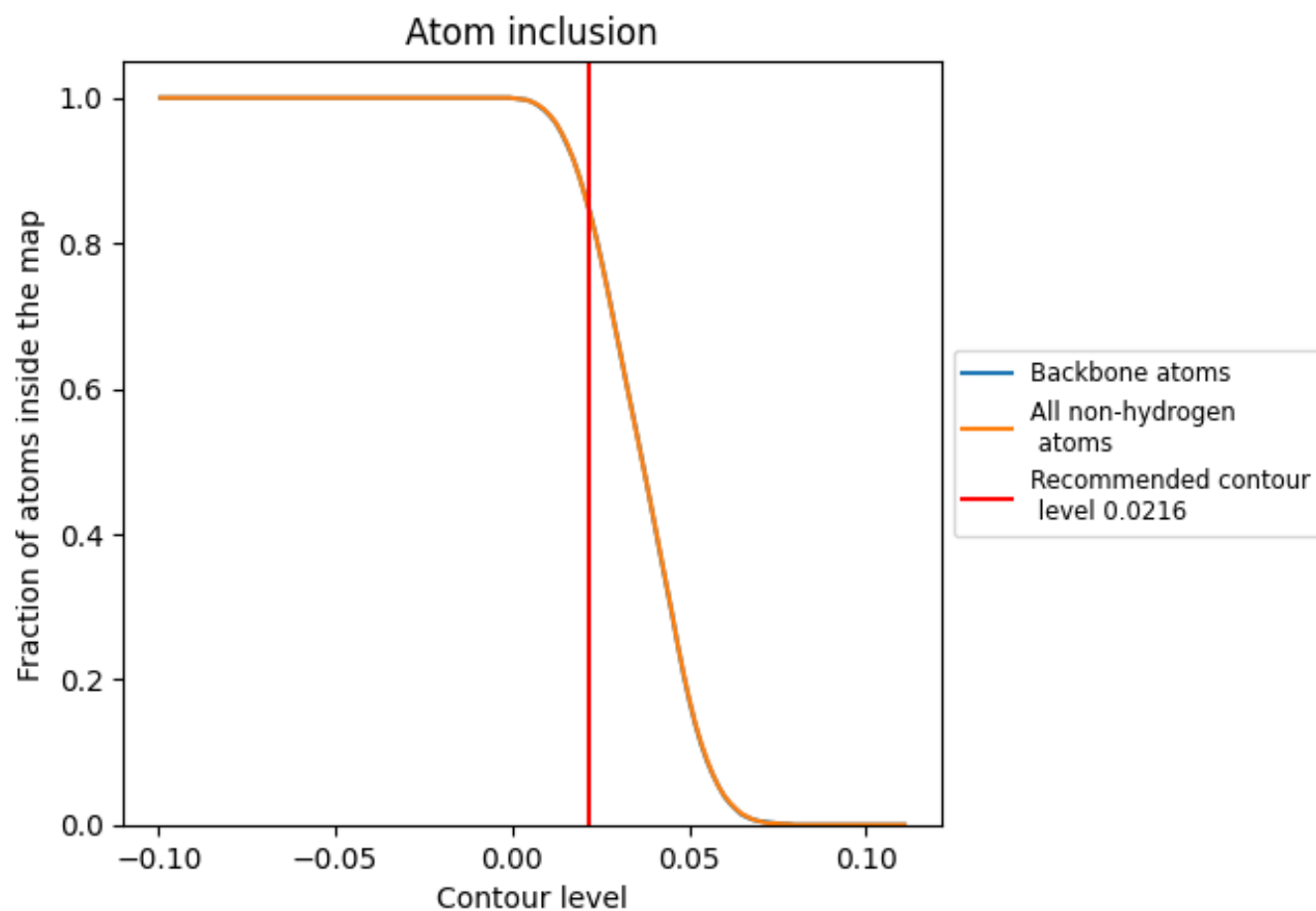
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0216).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0216) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8480   |  0.5020   |
| 1     |  0.8200   |  0.4290   |
| 2     |  0.5540   |  0.4150   |
| 3     |  0.7120   |  0.3890   |
| 4     |  0.6820   |  0.3790   |
| 5     |  0.5890   |  0.3710   |
| 6     |  0.5770   |  0.3260   |
| 7     |  0.5970   |  0.3490   |
| 8     |  0.6220   |  0.3830   |
| A     |  0.8600   |  0.5100   |
| B     |  0.8450   |  0.4910   |
| C     |  0.8450   |  0.4920   |
| D     |  0.8810   |  0.5240   |
| E     |  0.8630   |  0.5010   |
| F     |  0.8680  |  0.5070  |
| G     |  0.8690 |  0.5070 |
| H     |  0.8820 |  0.5290 |
| I     |  0.8610 |  0.5050 |
| J     |  0.8700 |  0.5180 |
| K     |  0.8610 |  0.4990 |
| L     |  0.8600 |  0.4990 |
| M     |  0.8080 |  0.4860 |
| N     |  0.7300 |  0.4460 |
| O     |  0.8910 |  0.5260 |
| P     |  0.8900 |  0.5220 |
| Q     |  0.5870 |  0.3250 |
| R     |  0.7080 |  0.4060 |
| S     |  0.7770 |  0.4120 |
| T     |  0.4940 |  0.2850 |

